



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 06:51 PM GMT

PDB ID : 4G5W
Title : Crystal Structure of the 70S ribosome with tigecycline. This entry contains the 50S subunit of molecule B.
Authors : Jenner, L.; Yusupov, M.; Yusupova, G.
Deposited on : 2012-07-18
Resolution : 3.10 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

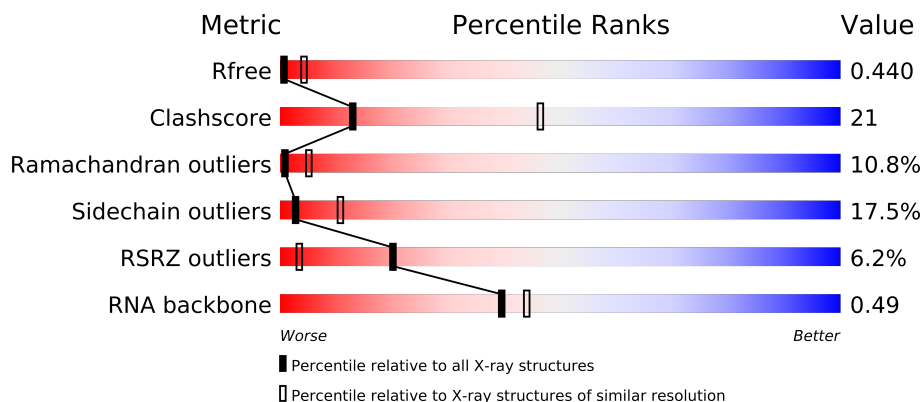
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1007 (3.18-3.02)
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)
RSRZ outliers	66119	1008 (3.18-3.02)
RNA backbone	1838	1047 (3.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	2912	
2	B	122	
3	D	276	
4	E	206	
5	F	210	
6	G	182	
7	H	180	
8	K	148	
9	M	140	
10	N	122	
11	O	150	
12	P	141	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
13	0	118	
14	Q	112	
15	R	146	
16	1	118	
17	2	101	
18	S	113	
19	T	96	
20	U	110	
21	V	206	
22	3	85	
23	Z	98	
24	W	72	
25	X	60	
26	4	71	
27	5	60	
28	6	54	
29	7	49	
30	8	65	

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 92006 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2906	Total	C	N	O	P	0	0	0
			62587	27857	11709	20116	2905			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	166	U	-	INSERTION	GB AP008226.1
A	654A	A	G	CONFLICT	GB AP008226.1
A	654E	C	G	CONFLICT	GB AP008226.1
A	654P	G	C	CONFLICT	GB AP008226.1
A	654T	A	C	CONFLICT	GB AP008226.1
A	1058	U	G	CONFLICT	GB AP008226.1
A	1080	A	C	CONFLICT	GB AP008226.1

- Molecule 2 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	208	Total	C	N	O	S	0	0	0
			1627	1037	304	283	3			

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	170	Total	C	N	O	S	0	0	0
			1307	829	245	232	1			

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	K	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	M	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	N	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	O	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	P	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	0	117	Total	C	N	O		0	0	0
			960	599	202	159				

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	Q	111	Total	C	N	O		0	0	0
			882	556	176	150				

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	R	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	1	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	2	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	S	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	T	92	Total	C	N	O	0	0	0
			725	471	131	123			

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	U	102	Total	C	N	O	S	0	0	0
			785	505	150	125	5			

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	V	179	Total	C	N	O	S	0	0	0
			1428	911	255	259	3			

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	3	77	Total	C	N	O	S	0	0	0
			613	379	129	104	1			

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	Z	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	W	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
25	X	59	Total	C	N	O	0	0	0
			469	298	90	81			

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	4	63	Total	C	N	O	S	0	0	0
			515	326	93	91	5			

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	6	45	Total	C	N	O	S	0	0	0
			389	241	79	65	4			

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			

- Molecule 30 is a protein called 50S ribosomal protein L35.

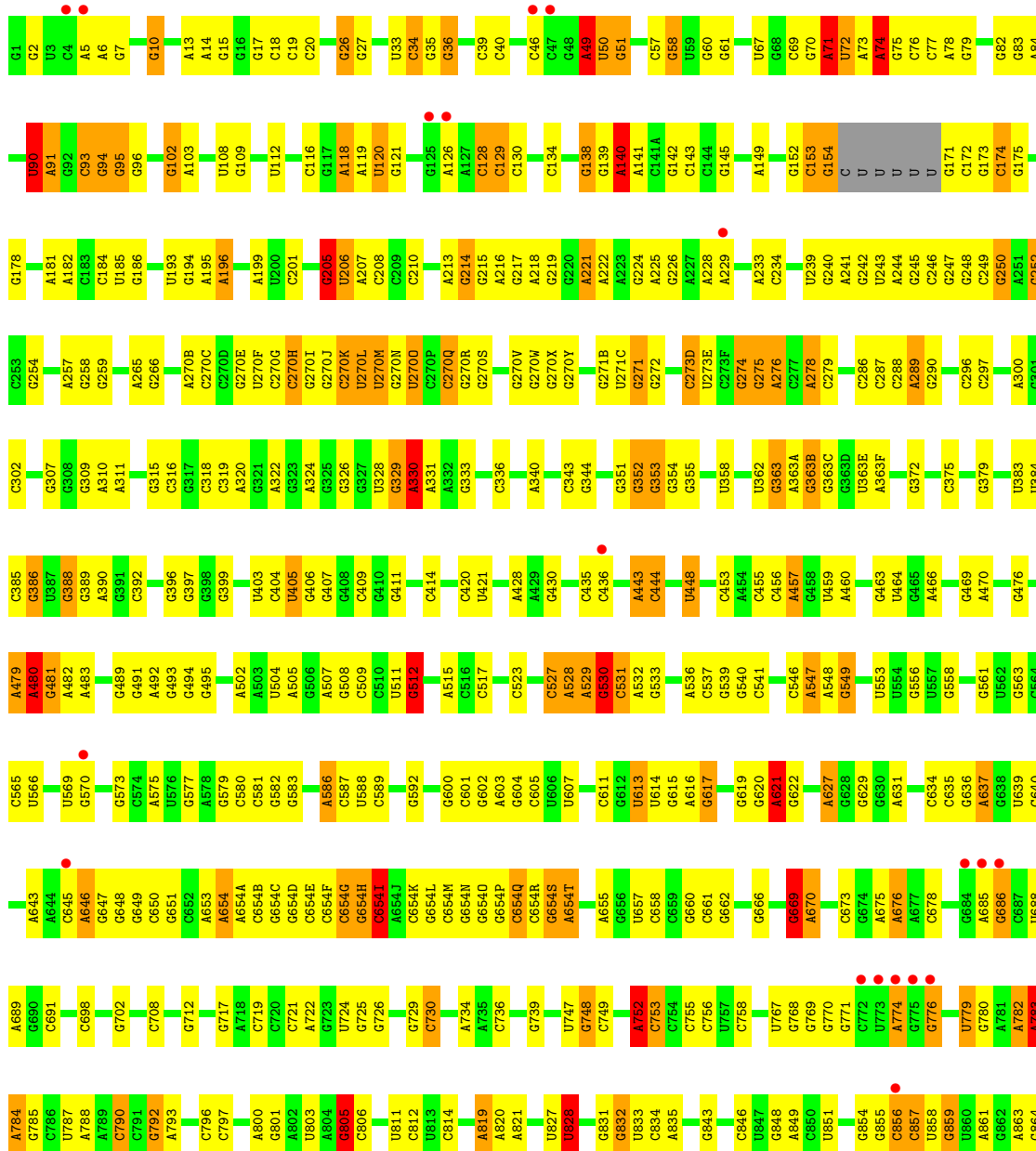
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	8	61	Total	C	N	O	S	0	0	0
			488	312	99	75	2			

3 Residue-property plots

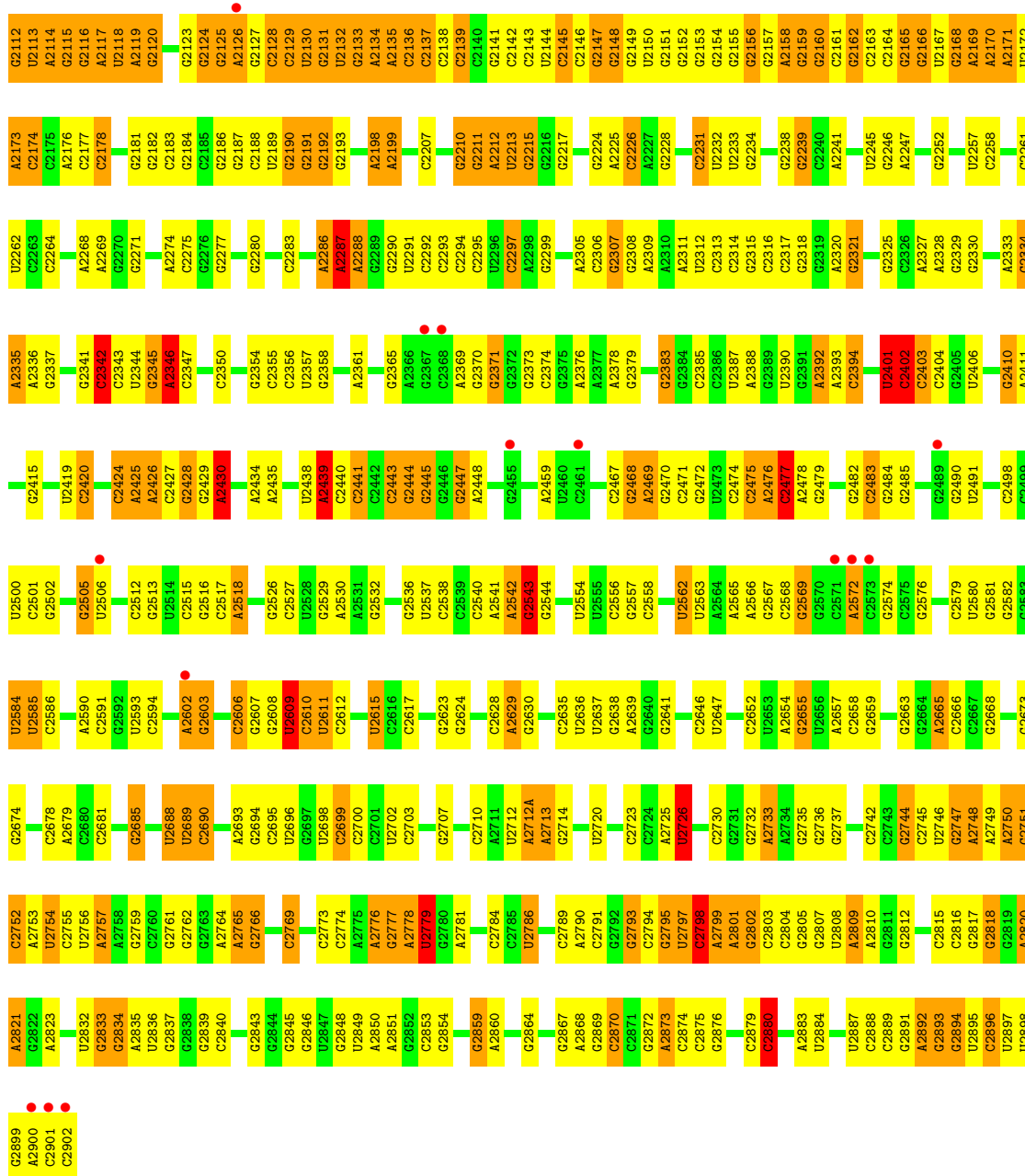
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 23S ribosomal RNA

Chain A: 

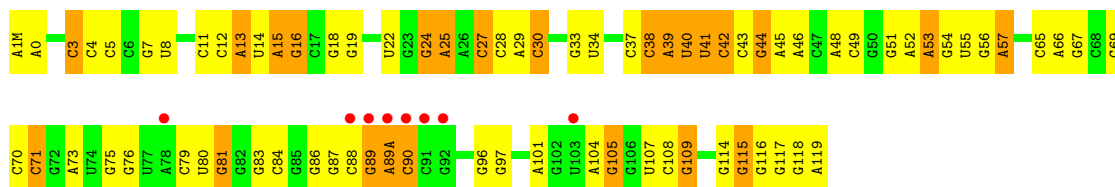


A2033	G1935	U1834	G1743	G1627	C1550	A1472	U1397	G1299	G1209	G1136	C1072	U1011	G932	C865
C2036	A1936	G1635	G1763	G1628	C1556	G1473	C1403	U1300	A1210	G1137	A1073	U1012	A933	A866
C2040	G1950	G1839	C1764	U1629	C1557	C1474	A1301	A1301	G1212	G1138	G1074	C1013	G934	G869
U2041	U1951	A1755	G1756	G1638	A1558	C1476	G1309	G1309	U1219	G1140	C1075	U1014	C935	G871
A2042	A1952	U1757	G1758	C1640	G1559	G1478	U1406	U1406	A1220	U1141	A1077	G1015	G938	U870
C2043	U1955	G1846	G1758	G1645	G1560	G1479	C1407	U1313	G1223	U1142	C1078	G1017	A872	A872
G2046	U1956	A1847	C1761	G1646	C1564	G1483	C1409	A1321	C1223	A1142A	A1080	U1019	A941	G873
G2049	C1962	G1848	A1762	G1647	C1565	G1484	G1410	A1322	G1224	A1143	U1081	U1019	G942	U877
G2052	U1963	G1850	G1763	C1648	A1566	G1486	A1412	U1323	C1225	C1145	U1082	A1020	U943	A878
G2053	G1964	U1851	G1764	G1651	A1567	G1487	G1414	G1324	G1228	G1149	U1083	U1023	A945	G879
A2054	C1965	C1852	G1771	G1652	G1568	G1488	G1415	G1325	C1230	C1150	A1085	G1024	G947	G881
C2055	A1966	A1853	G1772	G1653	A1569	U1489	U1415	U1326	G1236	G1151	A1086	U1025	G948	G882
G2056	C1967	A1570	A1773	A1654	A1570	G1490	G1416	C1327	G1236	A1155	A1088	U1026	G954	G883
A2059	A1970	U1576	U1779	G1655	U1576	G1491	G1417	U1328	U1239	A1156	G1089	A1028	G955	C884
A2060	A1971	C1577	A1780	C1656	C1577	G1492	A1419	C1330	G1240	G1157	U1090	A1028	G956	C885
A2062	A1972	U1578	A1781	C1657	U1578	A1493	U1420	A1331	U1240	C1158	G1091	A1030	G957	C886
C2065	G1989	C1658	G1781	C1658	A1580	A1496	G1424	G1338	G1245	U1165	A1098	U1033	U958	C887
C2066	C1990	G1659	C1782	U1671	G1581	U1497	G1428	A1342	C1251	C1166	G1099	G1034	U959	C888
G2067	U1991	C1660	A1582	G1672	A1582	A1505	A1427	A1349	G1252	C1161	U1105	U1034	A960	C889
C2068	G1989	G1666	A1583	U1672	C1585	C1506	C1428	A1349	A1253	G1162	C1100	G1035	G961	C890
G2069	C1992	G1673	A1584	G1673	A1584	C1509	A1434	A1349	G1254	C1161	U1101	U1035	C962	C892
C2070	U1993	C1675	A1585	G1675	A1511	C1512	G1436	U1352	U1255	G1169	C1102	G1040	G974	C893
C2071	C1994	G1678	A1591	G1678	C1592	U1516	C1437	G1366	G1256	G1170	A1103	G1042	C975	C894
U2079	U1995	U1678	C1592	U1678	G1593	U1517	G1441	U1367	C1257	G1171	C1104	G1043	C976	A899
G2080	C1996	U1688	G1594	U1688	A1594	U1518	G1442	G1368	G1257	G1173	U1105	G1044	C977	A900
C2081	C1999	A1689	G1595	A1689	A1595	C1518	A1444A	A1360	A1262	U1175	G1106	A1045	G977	A901
G2083	C2006	G1695	A1596	G1695	A1596	U1519	G1447	C1363	G1266	A1177	G1107	A1048	A980	C902
C2084	G2007	G1696	A1597	G1696	A1597	U1520	G1448	U1363	A1269	C1178	G1110	C1049	A883	C903
G2085	C2008	G1697	C1599	G1697	C1599	G1521	G1448	G1364	A1289	C1179	A1111	A1050	A984	C904
G2087	G2009	A1698	C1600	G1698	C1600	G1522	A1449	A1365	G1270	U1180	G1112	C1051	C985	U905
C2093	G2012	G1699	G1601	G1699	G1601	G1525	G1450	G1368	G1271	C1181	U1113	C1052	A909	G906
G2094	A2013	A1700	A1602	G1700	A1602	G1526	C1451	U1372	U1273	A1182	G1114	C1053	A988	A910
C2095	A2014	A1701	A1603	A1701	A1603	G1527	U1453	U1372	A1274	G1183	G1115	A1054	G989	A911
U2096	A2015	U1716	C1607	U1716	C1607	A1528	U1454	G1366	A1275	C1184	G1116	G1055	A990	C912
C2097	U2016	G1717	A1608	G1717	A1608	C1533	G1455	A1379	A1276	G1185	G1117	G1056	G993	U913
U2098	G2017	G1718	A1609	G1718	A1609	G1534	C1458	G1380	G1277	G1186	C1118	A1057	C914	C914
G2100	G2018	G1725	A1610	G1725	A1610	U1535	C1459	G1381	A1278	G1187	C1119	U1058	C994	C915
C2101	A2020	G1726	C1611	G1726	C1611	A1536	A1460	U1384	G1280	U1189	G1122	U1060	C995	G916
U2102	G2023	G1727	A1614	G1727	A1614	C1537	G1461	G1385	G1286	G1190	G1123	U1061	A996	A917
C2103	G2024	U1729	C1615	U1729	C1615	G1538	C1462	G1386	A1287	G1191	C1124	G1062	G997	A918
G2104	U1915	A1730	A1616	G1730	A1616	G1539	C1463	G1389	U1288	G1192	G1125	G1063	C998	G919
C2105	A1916	G1731	C1617	G1731	C1617	G1540	C1464	G1389	U1288	C1201	A1126	C1064	U999	G920
G2106	U1917	A1732	A1618	G1732	A1618	U1541	G1465	G1392	U1292	G1202	A1128	U1065	A1001	G921
C2107	G2027	G1735	G1622	U1735	G1622	A1542	C1467	A1392	U1292	G1203	A1129	U1066	C923	C923
G2108	G2029	C1735	A1622	G1735	A1622	A1543	C1467	A1393	C1293	G1204	U1130	G1068	C1005	A926
U2109	A2030	G1741	A1544	C1741	A1544	A1545	G1470	A1394	U1295	A1205	G1131	A1069	C1006	G928
G2110	G2032	C1742	G1626	C1742	G1626	A1545A	A1471	A1396	C1296	C1208	G1135	A1070	C1007	G929
C2111													A1010	



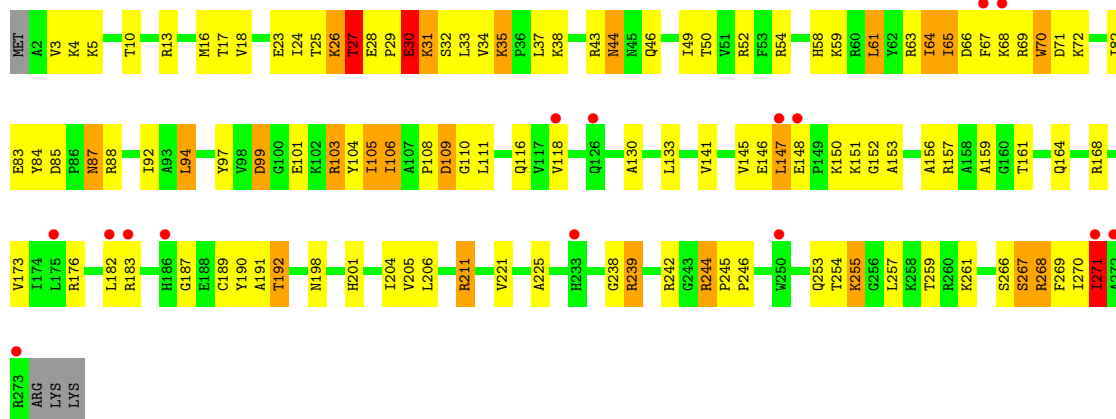
• Molecule 2: 5S RIBOSOMAL RNA

Chain B:



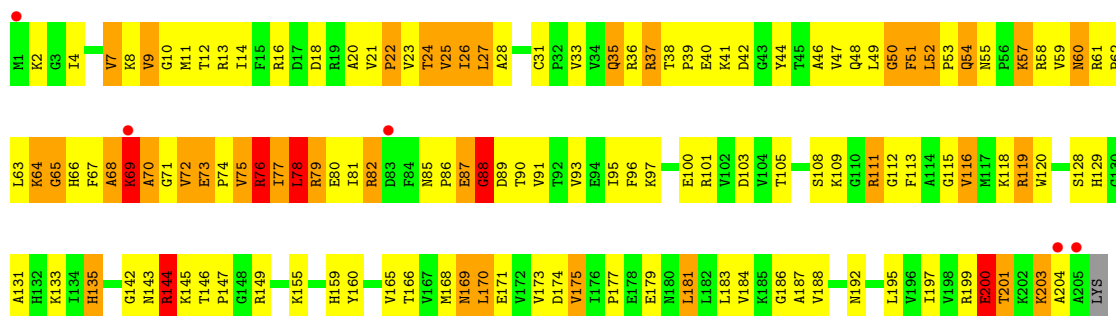
• Molecule 3: 50S ribosomal protein L2

Chain D:



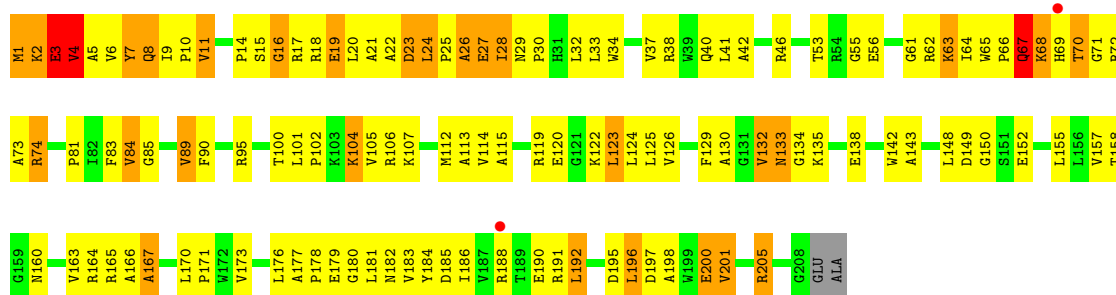
• Molecule 4: 50S ribosomal protein L3

Chain E:



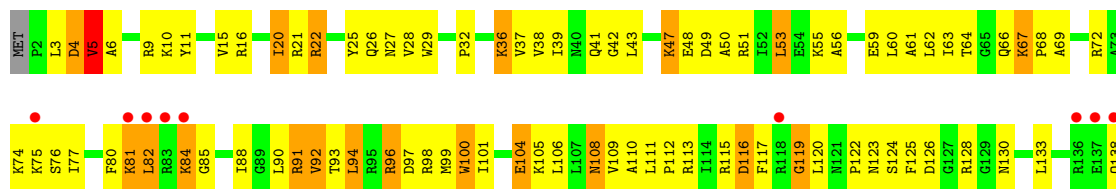
• Molecule 5: 50S ribosomal protein L4

Chain F:



• Molecule 6: 50S ribosomal protein L5

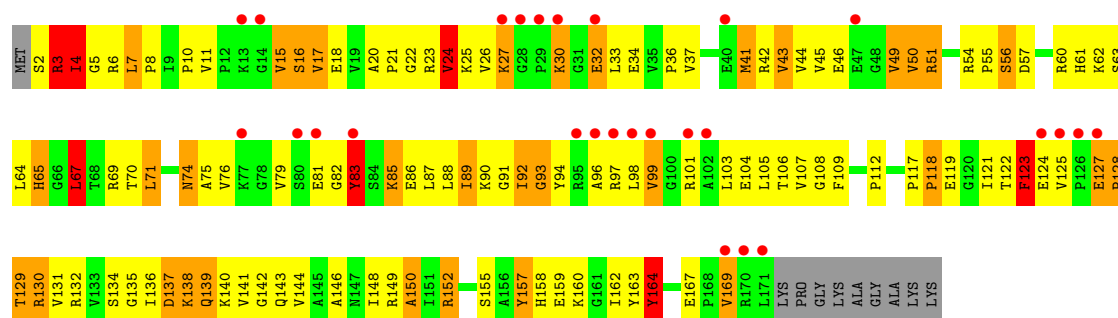
Chain G:





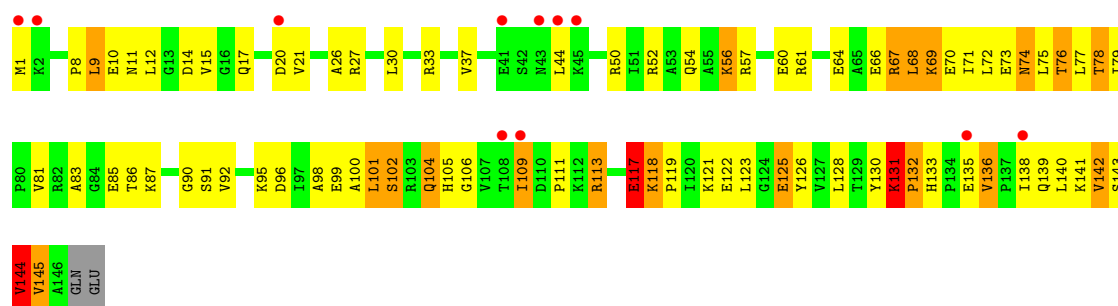
• Molecule 7: 50S ribosomal protein L6

Chain H:



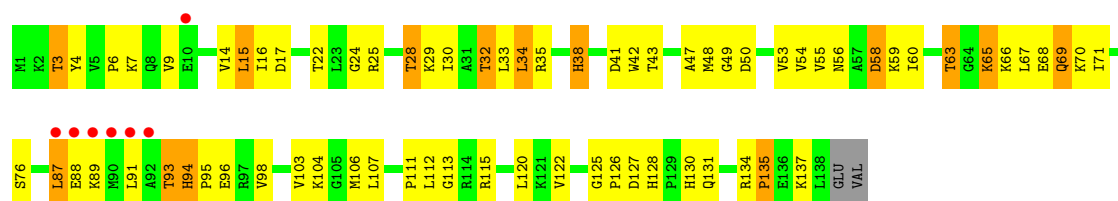
• Molecule 8: 50S ribosomal protein L9

Chain K:



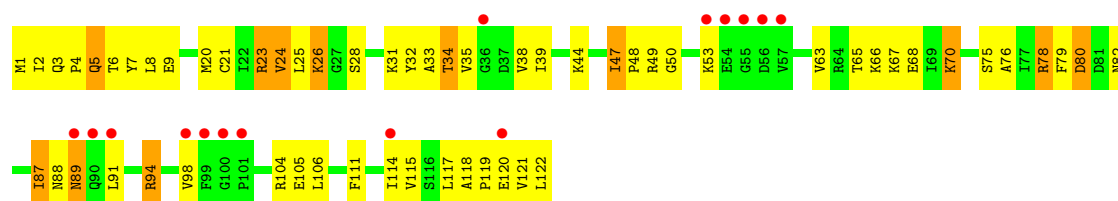
• Molecule 9: 50S ribosomal protein L13

Chain M:

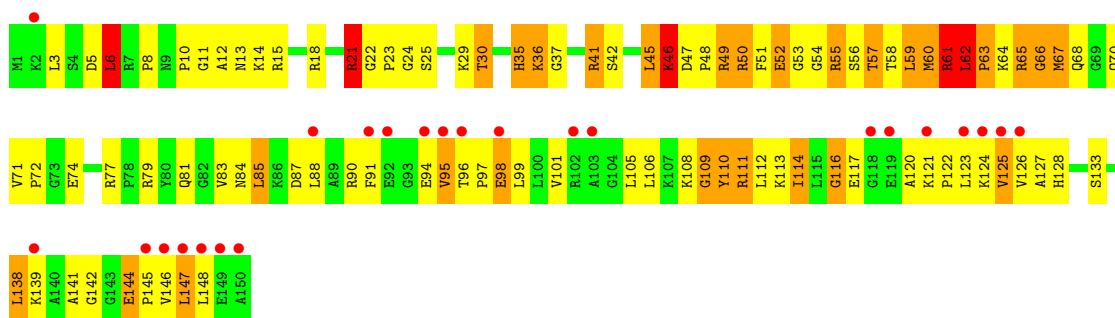


• Molecule 10: 50S ribosomal protein L14

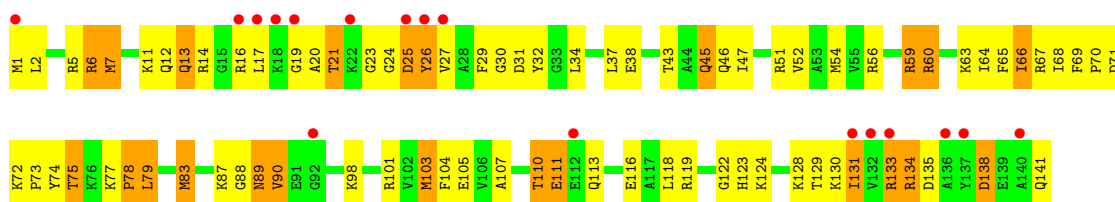
Chain N:



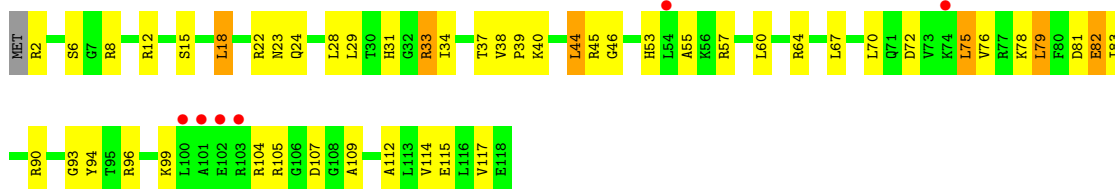
• Molecule 11: 50S ribosomal protein L15

Chain O: 

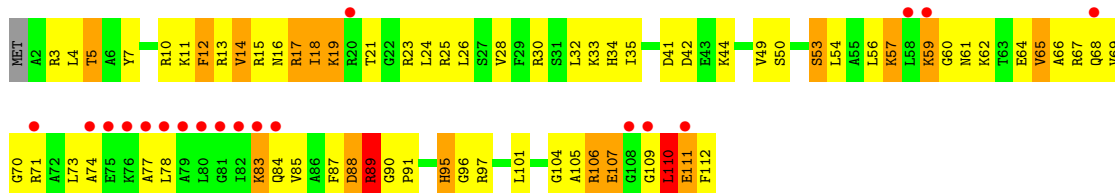
- Molecule 12: 50S ribosomal protein L16

Chain P: 

- Molecule 13: 50S ribosomal protein L17

Chain 0: 

- Molecule 14: 50S ribosomal protein L18

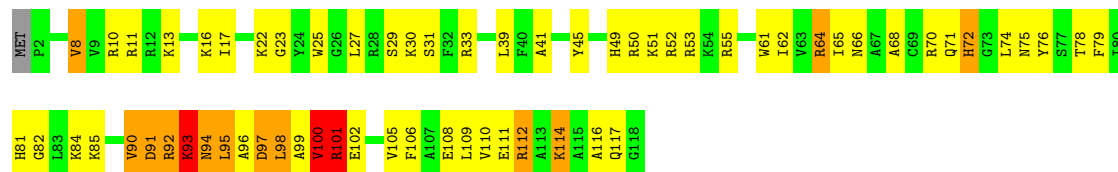
Chain Q: 

- Molecule 15: 50S ribosomal protein L19

Chain R: 

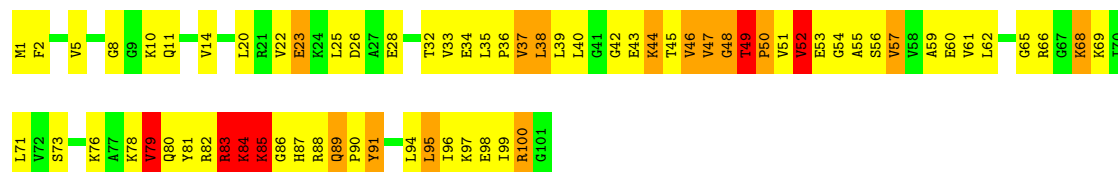
- Molecule 16: 50S ribosomal protein L20

Chain 1:



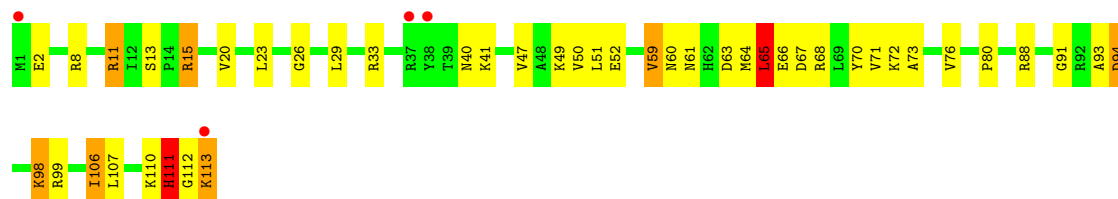
- Molecule 17: 50S ribosomal protein L21

Chain 2:



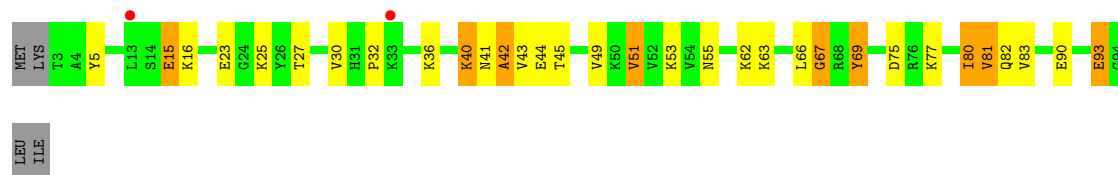
- Molecule 18: 50S ribosomal protein L22

Chain S:



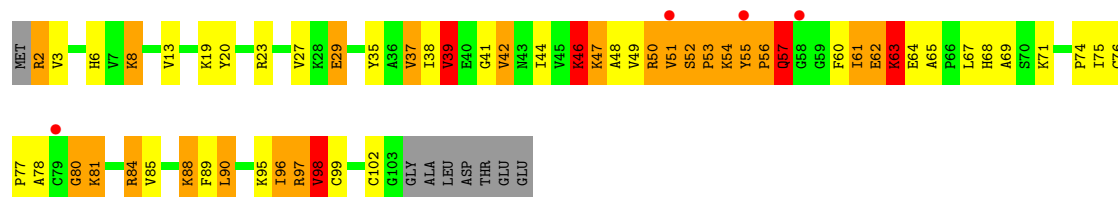
- Molecule 19: 50S ribosomal protein L23

Chain T:



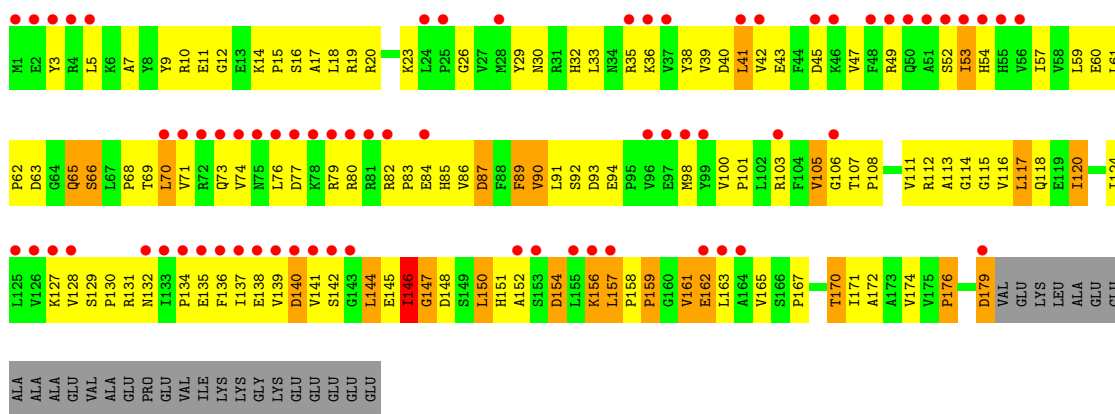
- Molecule 20: 50S ribosomal protein L24

Chain U:



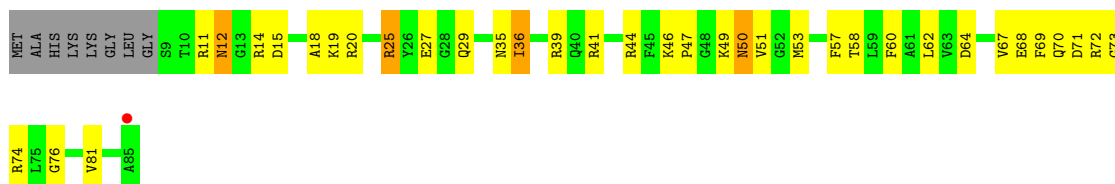
- Molecule 21: 50S ribosomal protein L25

Chain V:



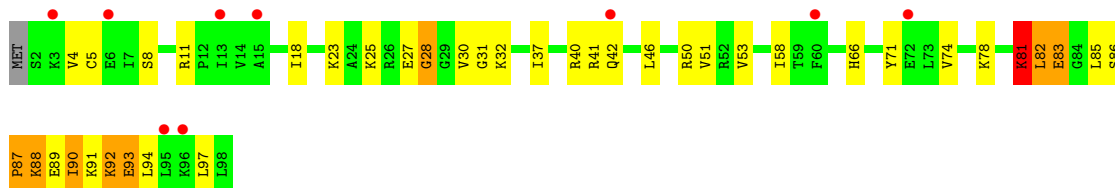
• Molecule 22: 50S ribosomal protein L27

Chain 3:



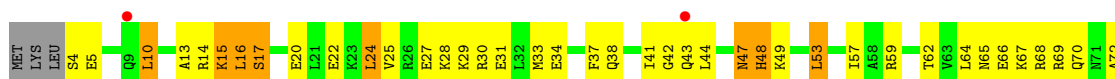
• Molecule 23: 50S ribosomal protein L28

Chain Z:



• Molecule 24: 50S ribosomal protein L29

Chain W:



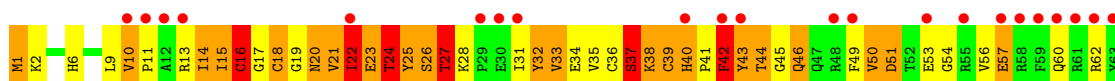
• Molecule 25: 50S ribosomal protein L30

Chain X:



• Molecule 26: 50S ribosomal protein L31

Chain 4:



GLY
ASP
SER
TYR
ARG
LYS
GLY
ARG

- Molecule 27: 50S ribosomal protein L32

Chain 5: 

MET A2 K3 H4 P5 V6 P7 K10 R15 R16 D17 A18 R19 H23 A24 L25 T29 C33 P34 E35 C36 K37 V45 C46 P47 E48 C49 G50 Y51 R55 K56 V57 L58 E59 V60

- Molecule 28: 50S ribosomal protein L33

Chain 6: 

MET ALA SER GLU VAL ARG ILE LYS L9 L10 L11 E12 C13 T14 E15 C16 R17 R18 R19 R20 R21 R22 R23 R24 R25 R26 R27 R28 R29 R30 R31 R32 R33 R34 R35 R36 R37 R38 Y39 C40 P41 V42 C43 R44 K45 H46 T47 V48 H49 R50 E51 V52 K53 ILE

- Molecule 29: 50S ribosomal protein L34

Chain 7: 

M1 T4 W5 Q6 P7 R8 R9 R10 K11 T14 T15 F18 R19 A20 R21 R22 R23 T24 K32 K33 R34 R35 R36 R37 R38 R39 W40 R41 L42 T43 P44 A45 V46 R47 R48 R49

- Molecule 30: 50S ribosomal protein L35

Chain 8: 

MET P2 K3 M4 K5 T6 H7 K8 R13 I16 V22 V23 A24 M25 T27 G28 K29 R30 R31 R32 R33 R34 Q35 K36 S37 G38 K39 E40 I41 Q42 Q43 K44 K47 F48 V49 L50 A51 K52 P53 E54 A55 E56 R57 I58 K59 L60 L61 L62 PRO TYR GLU

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.06Å 450.27Å 616.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	153.59 – 3.10 254.47 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (153.59-3.10) 93.4 (254.47-3.10)	Depositor EDS
R_{merge}	0.47	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 3.07Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_987)	Depositor
R, R_{free}	0.213 , 0.269 0.430 , 0.440	Depositor DCC
R_{free} test set	921 reflections (0.09%)	DCC
Wilson B-factor (Å ²)	81.8	Xtriage
Anisotropy	0.190	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 49.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 1045188 reflections	Xtriage
F_o, F_c correlation	0.67	EDS
Total number of atoms	92006	wwPDB-VP
Average B, all atoms (Å ²)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.61	4/70100 (0.0%)	1.09	282/109435 (0.3%)
2	B	0.55	0/2928	0.99	3/4568 (0.1%)
3	D	0.57	1/2165 (0.0%)	0.70	0/2919
4	E	0.50	0/1601	0.67	1/2160 (0.0%)
5	F	0.44	0/1662	0.64	0/2249
6	G	0.36	0/1499	0.59	0/2016
7	H	0.34	0/1332	0.70	1/1802 (0.1%)
8	K	0.40	0/1151	0.63	1/1558 (0.1%)
9	M	0.39	0/1131	0.58	0/1525
10	N	0.46	0/943	0.61	0/1269
11	O	0.42	0/1162	0.71	0/1544
12	P	0.45	0/1143	0.63	0/1527
13	O	0.46	0/974	0.63	0/1302
14	Q	0.44	0/892	0.73	1/1187 (0.1%)
15	R	0.43	0/1155	0.60	0/1542
16	1	0.42	0/982	0.64	0/1306
17	2	0.42	0/790	0.69	1/1057 (0.1%)
18	S	0.47	0/911	0.59	0/1220
19	T	0.55	0/739	0.64	0/993
20	U	0.50	0/798	0.69	1/1064 (0.1%)
21	V	0.37	0/1460	0.67	1/1982 (0.1%)
22	3	0.46	0/621	0.61	0/827
23	Z	0.49	0/770	0.68	0/1022
24	W	0.48	0/583	0.71	1/771 (0.1%)
25	X	0.40	0/474	0.56	0/635
26	4	0.44	0/527	0.69	0/709
27	5	0.45	0/473	0.67	0/639
28	6	0.52	0/396	0.68	0/529
29	7	0.54	0/438	0.65	0/575
30	8	0.61	0/494	0.93	1/649 (0.2%)
All	All	0.57	5/100294 (0.0%)	1.00	294/150581 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2430	A	N9-C4	-5.89	1.34	1.37
1	A	2518	A	N9-C4	-5.88	1.34	1.37
1	A	2443	C	N1-C6	-5.46	1.33	1.37
1	A	1992	G	N9-C4	5.06	1.42	1.38
3	D	30	GLU	CG-CD	5.02	1.59	1.51

All (294) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2401	U	C5-C6-N1	10.78	128.09	122.70
1	A	1786	A	C5-N7-C8	-10.44	98.68	103.90
1	A	1786	A	N7-C8-N9	10.20	118.90	113.80
1	A	2447	G	N1-C6-O6	9.54	125.62	119.90
1	A	2401	U	C5-C4-O4	-9.33	120.30	125.90
1	A	90	U	N3-C2-O2	-8.71	116.10	122.20
1	A	783	A	C5-N7-C8	-8.63	99.59	103.90
1	A	74	A	C2-N3-C4	-8.53	106.33	110.60
1	A	783	A	N1-C6-N6	8.50	123.70	118.60
1	A	2430	A	C2-N3-C4	-8.46	106.37	110.60
1	A	783	A	C4-C5-N7	8.43	114.91	110.70
1	A	90	U	C2-N1-C1'	8.34	127.71	117.70
1	A	801	G	N1-C6-O6	-8.31	114.91	119.90
1	A	90	U	N1-C2-O2	8.17	128.52	122.80
1	A	676	A	C2-N3-C4	-8.13	106.53	110.60
1	A	1992	G	N3-C4-C5	-8.06	124.57	128.60
1	A	130	C	C6-N1-C2	8.00	123.50	120.30
1	A	2477	C	N1-C2-O2	7.97	123.68	118.90
1	A	774	A	C2-N3-C4	-7.87	106.66	110.60
1	A	2699	C	C6-N1-C2	7.85	123.44	120.30
1	A	2430	A	N1-C6-N6	7.80	123.28	118.60
1	A	2688	U	N3-C2-O2	-7.75	116.77	122.20
1	A	828	U	N1-C2-O2	7.72	128.21	122.80
1	A	2067	G	C8-N9-C4	-7.72	103.31	106.40
1	A	530	G	C4-C5-N7	7.60	113.84	110.80
1	A	2477	C	C2-N1-C1'	7.54	127.10	118.80
1	A	1332	G	N7-C8-N9	7.52	116.86	113.10
1	A	1786	A	C6-C5-N7	-7.48	127.06	132.30
1	A	2401	U	C2-N1-C1'	7.47	126.67	117.70
1	A	1992	G	C8-N9-C4	-7.46	103.42	106.40
1	A	676	A	C5-N7-C8	-7.43	100.19	103.90
1	A	1786	A	C2-N3-C4	-7.41	106.89	110.60
1	A	1980	G	C8-N9-C4	-7.37	103.45	106.40
1	A	2287	A	C2-N3-C4	-7.31	106.94	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2426	A	C8-N9-C4	-7.28	102.89	105.80
1	A	1786	A	C4-C5-N7	7.25	114.33	110.70
1	A	2873	A	N7-C8-N9	7.25	117.42	113.80
1	A	121	G	C5-C6-O6	-7.21	124.27	128.60
1	A	405	U	C2-N1-C1'	7.20	126.34	117.70
1	A	530	G	C6-C5-N7	-7.20	126.08	130.40
1	A	49	A	C8-N9-C4	-7.15	102.94	105.80
1	A	2518	A	C2-N3-C4	-7.15	107.03	110.60
1	A	1332	G	C8-N9-C4	-7.13	103.55	106.40
1	A	2067	G	N9-C4-C5	7.12	108.25	105.40
1	A	2056	G	C5-C6-O6	-7.11	124.33	128.60
1	A	140	A	C5-N7-C8	-7.10	100.35	103.90
1	A	2873	A	C5-N7-C8	-7.09	100.36	103.90
1	A	828	U	N3-C2-O2	-7.07	117.25	122.20
1	A	140	A	N7-C8-N9	7.02	117.31	113.80
1	A	530	G	C5-C6-O6	-6.99	124.41	128.60
1	A	767	U	C5-C4-O4	6.95	130.07	125.90
1	A	2713	A	C5-N7-C8	-6.92	100.44	103.90
1	A	1021	A	C2-N3-C4	-6.92	107.14	110.60
1	A	2477	C	N3-C2-O2	-6.91	117.06	121.90
1	A	1698	A	C2-N3-C4	-6.88	107.16	110.60
1	A	2688	U	C5-C6-N1	-6.84	119.28	122.70
1	A	530	G	N1-C6-O6	6.83	124.00	119.90
1	A	2241	A	N1-C6-N6	-6.83	114.50	118.60
1	A	1899	G	C2-N3-C4	-6.78	108.51	111.90
1	A	1332	G	C2-N3-C4	-6.76	108.52	111.90
1	A	528	A	C2-N3-C4	-6.74	107.23	110.60
1	A	1787	A	N9-C4-C5	-6.74	103.10	105.80
1	A	2444	G	N3-C2-N2	-6.74	115.18	119.90
1	A	2685	G	N3-C2-N2	-6.72	115.19	119.90
1	A	94	G	N9-C4-C5	6.71	108.09	105.40
1	A	2447	G	C5-C6-O6	-6.68	124.59	128.60
1	A	2873	A	C2-N3-C4	-6.67	107.26	110.60
1	A	1396	U	N3-C2-O2	-6.67	117.53	122.20
1	A	1313	U	C2-N1-C1'	6.67	125.70	117.70
1	A	783	A	C2-N3-C4	-6.63	107.28	110.60
1	A	1989	G	N3-C2-N2	-6.56	115.31	119.90
1	A	2609	U	C5-C6-N1	-6.55	119.43	122.70
1	A	1616	A	C5-N7-C8	-6.54	100.63	103.90
1	A	330	A	C2-N3-C4	-6.54	107.33	110.60
1	A	512	G	N9-C4-C5	6.52	108.01	105.40
1	A	1899	G	N1-C2-N2	-6.51	110.34	116.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	Q	110	LEU	CA-CB-CG	6.48	130.20	115.30
1	A	1786	A	N1-C6-N6	6.46	122.47	118.60
1	A	2779	U	N3-C2-O2	-6.45	117.68	122.20
1	A	2401	U	C4-C5-C6	-6.45	115.83	119.70
1	A	2070	G	N1-C6-O6	-6.42	116.05	119.90
1	A	530	G	N9-C4-C5	-6.42	102.83	105.40
1	A	805	G	C5-C6-O6	-6.39	124.77	128.60
1	A	121	G	N1-C6-O6	6.39	123.73	119.90
1	A	1787	A	C8-N9-C4	6.38	108.35	105.80
1	A	270(H)	C	C6-N1-C2	-6.37	117.75	120.30
7	H	67	LEU	CB-CG-CD1	-6.36	100.19	111.00
1	A	2713	A	N1-C6-N6	6.32	122.39	118.60
1	A	480	A	N3-C4-N9	6.31	132.45	127.40
1	A	774	A	N3-C4-C5	6.30	131.21	126.80
1	A	1332	G	N1-C2-N3	6.30	127.68	123.90
1	A	1616	A	N7-C8-N9	6.30	116.95	113.80
1	A	2859	G	C8-N9-C4	-6.30	103.88	106.40
1	A	792	G	N3-C4-C5	-6.29	125.45	128.60
1	A	1569	A	C8-N9-C4	-6.29	103.28	105.80
1	A	613	U	N3-C2-O2	-6.28	117.81	122.20
1	A	116	C	C6-N1-C2	-6.27	117.79	120.30
1	A	270(C)	C	C6-N1-C2	-6.26	117.80	120.30
1	A	767	U	N3-C2-O2	-6.25	117.82	122.20
1	A	2426	A	N7-C8-N9	6.23	116.92	113.80
1	A	94	G	C4-C5-N7	-6.21	108.32	110.80
1	A	1158	C	C6-N1-C2	-6.20	117.82	120.30
1	A	2286	A	C8-N9-C4	-6.20	103.32	105.80
1	A	2441	C	N3-C4-N4	-6.19	113.67	118.00
1	A	1565	C	C6-N1-C2	-6.18	117.83	120.30
1	A	2501	C	C2-N1-C1'	-6.18	112.01	118.80
1	A	1569	A	N9-C4-C5	6.15	108.26	105.80
1	A	270(Y)	G	C5-C6-O6	6.15	132.29	128.60
20	U	46	LYS	CB-CG-CD	-6.14	95.64	111.60
1	A	13	A	C8-N9-C4	-6.13	103.35	105.80
1	A	2870	C	C6-N1-C2	-6.12	117.85	120.30
1	A	749	C	C6-N1-C2	6.12	122.75	120.30
1	A	2441	C	N3-C2-O2	-6.08	117.64	121.90
1	A	138	G	C8-N9-C4	-6.07	103.97	106.40
1	A	2443	C	C4-C5-C6	6.06	120.43	117.40
1	A	140	A	N1-C6-N6	6.06	122.23	118.60
1	A	1898	U	N3-C4-C5	-6.06	110.97	114.60
1	A	1786	A	C8-N9-C4	-6.02	103.39	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2491	U	C6-N1-C2	6.02	124.61	121.00
1	A	2231	C	C6-N1-C2	5.99	122.70	120.30
1	A	792	G	C8-N9-C4	-5.99	104.00	106.40
1	A	205	G	N3-C4-C5	-5.97	125.62	128.60
1	A	90	U	C6-N1-C2	-5.96	117.42	121.00
1	A	2518	A	N3-C4-C5	5.95	130.97	126.80
1	A	1902	C	N3-C4-C5	5.94	124.28	121.90
1	A	2795	G	N3-C4-C5	-5.94	125.63	128.60
1	A	1972	A	C8-N9-C4	5.94	108.17	105.80
30	8	31	HIS	CB-CA-C	5.92	122.24	110.40
1	A	1673	U	C5-C6-N1	-5.91	119.74	122.70
1	A	205	G	N3-C4-N9	5.89	129.53	126.00
1	A	570	G	C4-C5-N7	-5.88	108.45	110.80
1	A	2430	A	C5-C6-N1	-5.88	114.76	117.70
1	A	2726	U	C5-C4-O4	5.87	129.42	125.90
1	A	74	A	N1-C6-N6	5.86	122.12	118.60
1	A	2518	A	C5-N7-C8	-5.85	100.97	103.90
1	A	828	U	C2-N1-C1'	5.85	124.72	117.70
1	A	528	A	N1-C2-N3	5.84	132.22	129.30
1	A	2606	C	C2-N1-C1'	-5.81	112.41	118.80
1	A	776	G	C5-C6-O6	5.80	132.08	128.60
1	A	1558	A	C2-N3-C4	-5.79	107.70	110.60
1	A	2401	U	N3-C4-C5	5.79	118.07	114.60
1	A	479	A	N9-C4-C5	5.79	108.11	105.80
1	A	140	A	C4-C5-N7	5.78	113.59	110.70
1	A	1332	G	C5-N7-C8	-5.78	101.41	104.30
1	A	1528	A	N7-C8-N9	5.78	116.69	113.80
1	A	512	G	N3-C4-N9	-5.78	122.53	126.00
1	A	1251	C	N3-C4-C5	-5.77	119.59	121.90
17	2	37	VAL	CB-CA-C	-5.77	100.44	111.40
1	A	2401	U	C6-N1-C2	-5.75	117.55	121.00
1	A	929	G	N1-C6-O6	5.75	123.35	119.90
1	A	1564	C	C6-N1-C2	-5.74	118.01	120.30
1	A	621	A	C5-C6-N1	-5.73	114.83	117.70
1	A	2447	G	C6-C5-N7	-5.73	126.96	130.40
1	A	1980	G	N9-C4-C5	5.71	107.69	105.40
1	A	130	C	N3-C4-C5	5.71	124.18	121.90
1	A	2371	G	C4-C5-C6	5.68	122.21	118.80
1	A	2477	C	C6-N1-C2	-5.67	118.03	120.30
1	A	1902	C	N3-C4-N4	-5.67	114.03	118.00
1	A	1658	C	C2-N1-C1'	5.66	125.03	118.80
1	A	71	A	C5-N7-C8	-5.65	101.07	103.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2798	C	C6-N1-C2	-5.65	118.04	120.30
24	W	17	SER	C-N-CD	-5.64	108.19	120.60
1	A	669	G	N3-C4-C5	-5.63	125.78	128.60
1	A	676	A	C4-C5-N7	5.63	113.51	110.70
1	A	2713	A	C4-C5-N7	5.62	113.51	110.70
1	A	736	C	N1-C2-O2	-5.62	115.53	118.90
1	A	405	U	N1-C2-O2	5.61	126.73	122.80
1	A	600	G	N3-C2-N2	-5.61	115.97	119.90
1	A	676	A	N7-C8-N9	5.61	116.60	113.80
1	A	783	A	N7-C8-N9	5.61	116.60	113.80
1	A	933	A	N1-C6-N6	5.60	121.96	118.60
1	A	2443	C	N3-C4-C5	-5.59	119.66	121.90
1	A	512	G	C5-C6-O6	5.58	131.95	128.60
1	A	1950	G	C4-N9-C1'	5.58	133.75	126.50
1	A	2688	U	C4-C5-C6	5.58	123.05	119.70
1	A	783	A	C6-C5-N7	-5.56	128.41	132.30
1	A	2779	U	N1-C2-O2	5.56	126.69	122.80
1	A	2610	C	N1-C2-O2	5.54	122.23	118.90
1	A	2447	G	P-O3'-C3'	5.54	126.35	119.70
1	A	1342	A	C2-N3-C4	-5.54	107.83	110.60
1	A	1396	U	N1-C2-O2	5.53	126.67	122.80
1	A	1899	G	N1-C2-N3	5.53	127.22	123.90
1	A	74	A	N1-C2-N3	5.52	132.06	129.30
2	B	38	C	N1-C2-O2	-5.52	115.59	118.90
1	A	1950	G	N7-C8-N9	5.51	115.86	113.10
1	A	933	A	C5-N7-C8	-5.50	101.15	103.90
1	A	678	C	C6-N1-C2	5.49	122.50	120.30
1	A	1088	A	C8-N9-C4	-5.49	103.61	105.80
1	A	2606	C	C5-C6-N1	-5.48	118.26	121.00
1	A	1698	A	C5-C6-N1	-5.47	114.97	117.70
1	A	621	A	C5-N7-C8	-5.47	101.17	103.90
1	A	1900	A	C8-N9-C4	-5.46	103.62	105.80
1	A	1675	C	C6-N1-C2	5.45	122.48	120.30
1	A	570	G	C5-C6-O6	5.45	131.87	128.60
1	A	2818	G	C8-N9-C4	5.45	108.58	106.40
1	A	2134	A	N1-C6-N6	-5.44	115.33	118.60
1	A	2239	G	N1-C2-N2	-5.44	111.31	116.20
1	A	790	C	C6-N1-C2	5.43	122.47	120.30
1	A	2441	C	C5-C4-N4	5.43	124.00	120.20
1	A	1698	A	C5-N7-C8	-5.43	101.18	103.90
1	A	479	A	C8-N9-C4	-5.43	103.63	105.80
1	A	2779	U	C2-N1-C1'	5.43	124.21	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	480	A	N1-C2-N3	5.42	132.01	129.30
1	A	963	U	N3-C2-O2	-5.42	118.41	122.20
1	A	26	G	C8-N9-C4	-5.42	104.23	106.40
1	A	2500	U	N3-C4-O4	-5.42	115.61	119.40
1	A	2609	U	C2-N3-C4	-5.41	123.76	127.00
1	A	2286	A	N7-C8-N9	5.40	116.50	113.80
1	A	805	G	N9-C4-C5	-5.40	103.24	105.40
1	A	2515	C	N3-C2-O2	-5.39	118.12	121.90
1	A	1956	U	N3-C2-O2	-5.38	118.43	122.20
1	A	921	G	C8-N9-C4	-5.38	104.25	106.40
1	A	479	A	C8-N9-C1'	5.38	137.38	127.70
1	A	2056	G	N1-C6-O6	5.38	123.13	119.90
1	A	541	C	C6-N1-C2	-5.37	118.15	120.30
2	B	71	C	C6-N1-C2	-5.37	118.15	120.30
1	A	2371	G	C5-N7-C8	5.36	106.98	104.30
1	A	621	A	C2-N3-C4	-5.35	107.92	110.60
1	A	1381	G	N1-C6-O6	-5.35	116.69	119.90
1	A	965	C	C6-N1-C2	-5.34	118.16	120.30
1	A	388	G	C8-N9-C4	-5.34	104.26	106.40
1	A	678	C	N3-C4-C5	5.34	124.03	121.90
1	A	1914	C	N1-C2-O2	5.32	122.09	118.90
1	A	2518	A	C4-C5-N7	5.32	113.36	110.70
1	A	736	C	N3-C2-O2	5.31	125.62	121.90
1	A	676	A	N1-C6-N6	5.31	121.79	118.60
1	A	210	C	C5-C6-N1	-5.31	118.35	121.00
1	A	383	U	C5-C6-N1	-5.31	120.05	122.70
1	A	90	U	C5-C6-N1	5.29	125.35	122.70
1	A	828	U	C5-C4-O4	5.29	129.07	125.90
1	A	1557	C	C6-N1-C2	5.29	122.42	120.30
1	A	2518	A	N1-C6-N6	5.29	121.77	118.60
1	A	619	G	C8-N9-C4	-5.29	104.28	106.40
1	A	2346	A	C2-N3-C4	-5.27	107.97	110.60
1	A	2873	A	C5-C6-N1	-5.26	115.07	117.70
1	A	1895	C	C6-N1-C2	-5.26	118.20	120.30
1	A	669	G	C3'-C2'-C1'	5.25	105.70	101.50
1	A	2562	U	C5-C6-N1	-5.25	120.08	122.70
1	A	783	A	N9-C4-C5	-5.24	103.70	105.80
1	A	1342	A	N7-C8-N9	5.24	116.42	113.80
1	A	2084	C	C6-N1-C2	5.22	122.39	120.30
1	A	2401	U	N1-C2-O2	5.21	126.45	122.80
1	A	570	G	N9-C4-C5	5.21	107.48	105.40
1	A	1695	G	C4-N9-C1'	5.20	133.26	126.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	270(K)	C	N1-C2-O2	5.20	122.02	118.90
1	A	453	C	C6-N1-C2	5.20	122.38	120.30
1	A	140	A	C6-C5-N7	-5.19	128.67	132.30
1	A	2439	A	P-O3'-C3'	5.19	125.92	119.70
1	A	201	C	C6-N1-C2	5.18	122.37	120.30
1	A	2685	G	N3-C4-N9	-5.18	122.89	126.00
1	A	1328	G	C5-C6-O6	-5.17	125.50	128.60
1	A	1786	A	C5-C6-N1	-5.17	115.12	117.70
1	A	2873	A	C8-N9-C4	-5.17	103.73	105.80
1	A	933	A	C4-C5-N7	5.17	113.28	110.70
1	A	2402	C	C4-C5-C6	5.16	119.98	117.40
1	A	2342	C	C6-N1-C2	-5.15	118.24	120.30
1	A	912	C	C6-N1-C2	-5.14	118.25	120.30
1	A	1171	G	P-O3'-C3'	5.12	125.85	119.70
1	A	1208	C	C6-N1-C2	-5.12	118.25	120.30
1	A	1614	A	N7-C8-N9	5.12	116.36	113.80
1	A	2390	U	C6-N1-C2	-5.11	117.94	121.00
21	V	147	GLY	N-CA-C	-5.10	100.36	113.10
2	B	39	A	C8-N9-C4	-5.09	103.76	105.80
4	E	88	GLY	N-CA-C	5.09	125.83	113.10
1	A	1653	G	C8-N9-C4	-5.09	104.36	106.40
1	A	691	C	N1-C2-O2	-5.08	115.85	118.90
1	A	2483	C	C6-N1-C2	-5.07	118.27	120.30
1	A	2606	C	C6-N1-C2	5.07	122.33	120.30
1	A	74	A	C5-C6-N1	-5.06	115.17	117.70
1	A	2070	G	C5-C6-O6	5.06	131.64	128.60
1	A	2490	G	N7-C8-N9	5.06	115.63	113.10
1	A	1407	C	C6-N1-C2	-5.06	118.28	120.30
1	A	611	C	C6-N1-C2	5.04	122.32	120.30
1	A	1248	G	C8-N9-C4	5.04	108.42	106.40
1	A	2880	C	C6-N1-C2	-5.04	118.28	120.30
1	A	2079	U	C4-C5-C6	5.04	122.72	119.70
1	A	512	G	C4-C5-N7	-5.04	108.78	110.80
1	A	270(K)	C	C2-N1-C1'	5.04	124.34	118.80
1	A	792	G	C4-C5-C6	5.03	121.82	118.80
1	A	748	G	N1-C6-O6	-5.03	116.88	119.90
1	A	1379	A	C4-C5-N7	5.03	113.22	110.70
1	A	2688	U	N1-C2-O2	5.03	126.32	122.80
1	A	1528	A	C8-N9-C4	-5.03	103.79	105.80
8	K	131	LYS	C-N-CD	-5.03	109.54	120.60
1	A	570	G	C8-N9-C4	-5.02	104.39	106.40
1	A	2015	A	N1-C6-N6	-5.02	115.59	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1277	G	C8-N9-C4	5.02	108.41	106.40
1	A	600	G	N1-C6-O6	5.02	122.91	119.90
1	A	752	A	C8-N9-C4	-5.02	103.79	105.80
1	A	2543	G	N7-C8-N9	5.02	115.61	113.10
1	A	669	G	N1-C2-N2	-5.01	111.69	116.20
1	A	783	A	N3-C4-C5	5.00	130.30	126.80
1	A	654(I)	C	C2-N1-C1'	5.00	124.30	118.80
1	A	805	G	N1-C6-O6	5.00	122.90	119.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	62587	0	31554	1344	0
2	B	2617	0	1328	85	0
3	D	2115	0	2195	141	0
4	E	1568	0	1634	207	0
5	F	1627	0	1680	130	0
6	G	1474	0	1535	101	0
7	H	1307	0	1382	122	0
8	K	1136	0	1223	44	0
9	M	1104	0	1180	50	0
10	N	933	0	996	41	0
11	O	1145	0	1228	155	0
12	P	1122	0	1179	59	0
13	0	960	0	1021	37	0
14	Q	882	0	943	72	0
15	R	1141	0	1202	62	0
16	1	964	0	1022	69	0
17	2	779	0	852	89	0
18	S	900	0	964	27	0
19	T	725	0	778	20	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	U	785	0	878	57	0
21	V	1428	0	1454	87	0
22	3	613	0	633	35	0
23	Z	763	0	848	34	0
24	W	581	0	629	30	0
25	X	469	0	518	19	0
26	4	515	0	510	71	0
27	5	459	0	480	24	0
28	6	389	0	404	76	0
29	7	430	0	480	13	0
30	8	488	0	560	71	0
All	All	92006	0	61290	2906	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 21.

All (2906) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:H:127:GLU:CG	7:H:128:PRO:HD3	1.36	1.54
4:E:11:MET:SD	4:E:24:THR:HG22	1.47	1.52
17:2:49:THR:HB	17:2:50:PRO:CD	1.45	1.47
3:D:34:VAL:HG22	3:D:35:LYS:CE	1.44	1.46
11:O:71:VAL:CG1	11:O:72:PRO:HD3	1.44	1.45
3:D:34:VAL:CG2	3:D:35:LYS:NZ	1.76	1.45
3:D:34:VAL:HG23	3:D:35:LYS:NZ	1.22	1.43
3:D:35:LYS:CD	3:D:64:ILE:HG23	1.52	1.35
11:O:62:LEU:HD11	30:8:25:MET:C	1.47	1.34
3:D:34:VAL:HG22	3:D:35:LYS:CD	1.62	1.28
3:D:34:VAL:CG2	3:D:35:LYS:CE	2.11	1.26
17:2:38:LEU:O	17:2:51:VAL:HG13	1.18	1.26
4:E:11:MET:SD	4:E:24:THR:CG2	2.26	1.24
4:E:11:MET:CG	4:E:24:THR:HG22	1.74	1.18
3:D:34:VAL:CG2	3:D:35:LYS:HZ3	1.45	1.18
28:6:15:GLU:HG2	28:6:16:CYS:N	1.45	1.17
11:O:71:VAL:HG12	11:O:72:PRO:CD	1.75	1.16
4:E:66:HIS:NE2	4:E:67:PHE:HD1	1.43	1.15
11:O:62:LEU:HD11	30:8:25:MET:O	1.41	1.14
3:D:35:LYS:HD2	3:D:64:ILE:CG2	1.76	1.14
3:D:35:LYS:HE3	3:D:64:ILE:O	1.45	1.13
4:E:78:LEU:O	4:E:79:ARG:HD2	1.50	1.12
11:O:49:ARG:HG2	11:O:49:ARG:O	1.49	1.11
17:2:49:THR:CB	17:2:50:PRO:HD2	1.81	1.10

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2114:A:N6	1:A:2119:A:N7	1.99	1.10
5:F:24:LEU:HB3	5:F:25:PRO:CD	1.82	1.09
7:H:127:GLU:CB	7:H:128:PRO:CD	2.30	1.09
26:4:39:CYS:C	26:4:41:PRO:HD3	1.71	1.09
11:O:71:VAL:CG1	11:O:72:PRO:CD	2.30	1.08
11:O:62:LEU:CD1	30:8:25:MET:O	2.00	1.08
7:H:127:GLU:CG	7:H:128:PRO:CD	2.30	1.08
5:F:24:LEU:HB3	5:F:25:PRO:HD2	1.09	1.07
11:O:64:LYS:HB3	30:8:25:MET:HG3	1.36	1.07
11:O:62:LEU:HD21	30:8:25:MET:O	1.54	1.07
20:U:52:SER:CA	20:U:56:PRO:HA	1.85	1.07
4:E:11:MET:HA	4:E:24:THR:HA	1.07	1.07
11:O:48:PRO:O	11:O:50:ARG:N	1.87	1.06
3:D:34:VAL:C	3:D:35:LYS:HD3	1.74	1.06
11:O:61:ARG:O	11:O:62:LEU:HB2	1.45	1.06
11:O:62:LEU:CG	30:8:25:MET:O	2.03	1.06
3:D:34:VAL:HG22	3:D:35:LYS:HD3	1.33	1.05
28:6:14:THR:HB	28:6:20:ASN:O	1.56	1.05
7:H:127:GLU:CB	7:H:128:PRO:HD3	1.83	1.05
20:U:52:SER:HA	20:U:56:PRO:CA	1.86	1.05
1:A:2638:G:P	4:E:82:ARG:HH22	1.78	1.05
4:E:9:VAL:HG21	4:E:25:VAL:CG1	1.87	1.04
3:D:35:LYS:HE3	3:D:64:ILE:HG12	1.36	1.04
4:E:60:ASN:HB3	4:E:63:LEU:HD11	1.36	1.03
17:2:49:THR:CB	17:2:50:PRO:CD	2.30	1.03
3:D:35:LYS:CD	3:D:35:LYS:N	2.21	1.03
20:U:50:ARG:HB3	20:U:53:PRO:HG3	1.05	1.03
5:F:21:ALA:O	5:F:24:LEU:HD23	1.56	1.02
26:4:40:HIS:HA	26:4:44:THR:O	1.59	1.02
17:2:39:LEU:HG	17:2:51:VAL:HG22	1.06	1.02
3:D:35:LYS:CE	3:D:64:ILE:O	2.06	1.02
11:O:64:LYS:O	11:O:64:LYS:HD3	1.59	1.02
17:2:39:LEU:HG	17:2:51:VAL:CG2	1.88	1.01
20:U:50:ARG:HB3	20:U:53:PRO:CG	1.89	1.01
26:4:38:LYS:HB2	26:4:38:LYS:HZ3	1.25	1.01
1:A:2638:G:OP2	4:E:82:ARG:NH2	1.93	1.01
1:A:2444:G:OP2	5:F:68:LYS:NZ	1.94	1.01
5:F:2:LYS:O	5:F:24:LEU:HG	1.62	1.00
20:U:52:SER:HA	20:U:56:PRO:HA	1.01	1.00
21:V:146:ILE:HD12	21:V:147:GLY:H	1.24	1.00
4:E:55:ASN:ND2	4:E:73:GLU:O	1.95	0.99
20:U:56:PRO:O	20:U:57:GLN:HB2	1.58	0.99

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:H:127:GLU:HG3	7:H:128:PRO:HD3	1.03	0.99
28:6:12:GLU:HG3	28:6:21:TYR:CD1	1.97	0.99
4:E:9:VAL:HG21	4:E:25:VAL:HG12	1.43	0.99
4:E:66:HIS:NE2	4:E:67:PHE:CD1	2.30	0.99
7:H:127:GLU:HB3	7:H:128:PRO:HD2	1.44	0.99
7:H:127:GLU:HG3	7:H:128:PRO:CD	1.90	0.98
5:F:3:GLU:HA	5:F:24:LEU:CG	1.91	0.98
1:A:2096:U:H3	1:A:2193:G:H1	1.11	0.98
6:G:112:PRO:HG2	26:4:37:SER:CB	1.94	0.98
6:G:112:PRO:CG	26:4:37:SER:HB2	1.92	0.98
3:D:34:VAL:HG22	3:D:35:LYS:HE2	1.46	0.98
11:O:62:LEU:CD2	30:8:25:MET:O	2.09	0.98
1:A:93:C:O5'	20:U:54:LYS:NZ	1.96	0.98
17:2:38:LEU:O	17:2:51:VAL:CG1	2.12	0.98
4:E:11:MET:CA	4:E:24:THR:HA	1.93	0.98
28:6:17:LYS:HD2	28:6:17:LYS:N	1.77	0.97
3:D:35:LYS:CE	3:D:64:ILE:HG12	1.94	0.97
7:H:127:GLU:HB3	7:H:128:PRO:CD	1.94	0.97
4:E:11:MET:HA	4:E:24:THR:CA	1.94	0.97
5:F:3:GLU:HA	5:F:24:LEU:CD1	1.95	0.97
26:4:16:CYS:SG	26:4:17:GLY:N	2.38	0.96
5:F:66:PRO:O	5:F:67:GLN:HB3	1.62	0.96
2:B:18:G:H1	2:B:65:C:H42	1.09	0.96
4:E:60:ASN:HD22	4:E:63:LEU:HD21	1.30	0.95
4:E:23:VAL:HA	4:E:184:VAL:O	1.66	0.94
17:2:49:THR:HB	17:2:50:PRO:HD3	1.49	0.94
1:A:1070:A:C8	1:A:1096:A:H1'	2.03	0.94
4:E:66:HIS:HE2	4:E:67:PHE:HD1	1.09	0.94
26:4:40:HIS:N	26:4:41:PRO:CD	2.30	0.94
17:2:91:TYR:HD2	17:2:91:TYR:C	1.71	0.94
17:2:47:VAL:HG22	17:2:47:VAL:O	1.66	0.94
1:A:330:A:H2	1:A:1210:A:HO2'	1.10	0.94
5:F:3:GLU:HA	5:F:24:LEU:HG	1.49	0.94
28:6:39:TYR:O	28:6:39:TYR:HD2	1.51	0.93
28:6:14:THR:O	28:6:49:HIS:HA	1.68	0.93
6:G:112:PRO:HG2	26:4:37:SER:HB2	0.98	0.93
1:A:93:C:H4'	20:U:54:LYS:HZ2	1.31	0.93
26:4:38:LYS:HB2	26:4:38:LYS:NZ	1.77	0.92
3:D:35:LYS:HD2	3:D:64:ILE:HG23	0.92	0.92
4:E:78:LEU:C	4:E:79:ARG:HD2	1.88	0.91
1:A:1054:A:N6	1:A:1105:U:O4	2.01	0.91
1:A:676:A:H8	1:A:2069:G:H21	1.18	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:F:26:ALA:O	5:F:27:GLU:HG3	1.70	0.91
20:U:52:SER:OG	20:U:56:PRO:HG3	1.70	0.91
11:O:62:LEU:H	11:O:63:PRO:HD3	1.35	0.91
5:F:24:LEU:CB	5:F:25:PRO:HD2	1.99	0.90
1:A:2061:G:OP1	5:F:68:LYS:HE3	1.71	0.90
3:D:49:ILE:HD11	3:D:52:ARG:HA	1.53	0.90
4:E:66:HIS:CE1	4:E:67:PHE:HB2	2.07	0.90
26:4:39:CYS:C	26:4:41:PRO:CD	2.40	0.89
1:A:1073:A:OP2	1:A:1094:U:N3	2.04	0.89
28:6:15:GLU:HG3	28:6:47:THR:CG2	2.03	0.89
17:2:39:LEU:CG	17:2:51:VAL:HG22	2.00	0.89
1:A:1169:G:H1	1:A:1180:C:H42	1.12	0.89
1:A:2807:G:N1	1:A:2893:G:O6	2.06	0.89
2:B:3:C:H42	2:B:117:G:H1	1.21	0.89
17:2:49:THR:HB	17:2:50:PRO:HD2	0.91	0.89
1:A:93:C:C5'	20:U:54:LYS:HZ1	1.85	0.89
28:6:39:TYR:C	28:6:39:TYR:CD2	2.47	0.88
12:P:75:THR:HG21	12:P:87:LYS:HE3	1.53	0.88
3:D:34:VAL:CG2	3:D:35:LYS:CD	2.49	0.88
4:E:63:LEU:O	4:E:64:LYS:HG2	1.72	0.88
4:E:13:ARG:HA	4:E:21:VAL:O	1.73	0.88
11:O:49:ARG:HD2	30:8:59:LYS:HG3	1.52	0.88
11:O:62:LEU:HD12	30:8:25:MET:HB2	1.54	0.88
28:6:15:GLU:HG2	28:6:16:CYS:H	1.05	0.88
3:D:34:VAL:CG2	3:D:35:LYS:HD3	2.05	0.87
11:O:64:LYS:HB3	30:8:25:MET:CG	2.05	0.87
1:A:617:G:OP1	5:F:40:GLN:NE2	2.07	0.87
4:E:9:VAL:CG2	4:E:25:VAL:HG12	2.05	0.86
11:O:47:ASP:HB3	11:O:48:PRO:CA	2.05	0.86
13:0:37:THR:HG22	13:0:39:PRO:HD2	1.57	0.86
17:2:91:TYR:C	17:2:91:TYR:CD2	2.47	0.86
20:U:50:ARG:CB	20:U:53:PRO:HG3	2.00	0.86
1:A:287:C:N4	1:A:354:G:O6	2.09	0.86
22:3:11:ARG:O	22:3:14:ARG:NH2	2.07	0.86
1:A:2777:G:H5''	1:A:2778:A:H5'	1.58	0.86
3:D:35:LYS:HD3	3:D:35:LYS:N	1.87	0.86
1:A:833:U:O2	11:O:55:ARG:NH1	2.09	0.86
30:8:32:LEU:HD12	30:8:34:TRP:H	1.41	0.86
28:6:44:ARG:HD3	28:6:47:THR:HG21	1.57	0.85
1:A:252:G:OP2	11:O:50:ARG:NH2	2.10	0.85
4:E:66:HIS:CD2	4:E:67:PHE:HD1	1.94	0.85
11:O:62:LEU:CD1	30:8:25:MET:C	2.38	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2379:G:O2'	14:Q:17:ARG:NH1	2.09	0.85
7:H:83:TYR:HA	7:H:134:SER:HB3	1.58	0.85
28:6:15:GLU:CG	28:6:16:CYS:N	2.34	0.84
10:N:115:VAL:HG13	10:N:121:VAL:HG21	1.59	0.84
1:A:2130:U:HO2'	1:A:2133:G:HO2'	1.12	0.84
1:A:1019:U:H3	1:A:1142(A):A:H62	1.25	0.84
1:A:2115:G:O3'	1:A:2165:G:N2	2.11	0.84
3:D:35:LYS:HD2	3:D:35:LYS:N	1.91	0.84
11:O:64:LYS:CB	30:8:25:MET:HG3	2.08	0.84
1:A:2292:C:OP1	14:Q:17:ARG:NH2	2.11	0.84
1:A:2125:G:N1	1:A:2172:U:OP1	2.10	0.83
5:F:3:GLU:HA	5:F:24:LEU:HD11	1.58	0.83
28:6:39:TYR:CE2	28:6:40:CYS:O	2.30	0.83
11:O:47:ASP:HB3	11:O:48:PRO:C	1.98	0.83
11:O:62:LEU:H	11:O:63:PRO:CD	1.90	0.83
28:6:15:GLU:HB2	28:6:47:THR:HG23	1.59	0.83
2:B:90:C:OP2	12:P:16:ARG:NH2	2.11	0.83
3:D:34:VAL:HG23	3:D:35:LYS:HZ2	1.01	0.82
28:6:39:TYR:O	28:6:39:TYR:CD2	2.32	0.82
1:A:654(B):C:N3	1:A:654(S):G:N1	2.25	0.82
1:A:1899:G:H21	1:A:1902:C:H41	1.24	0.82
11:O:71:VAL:HG13	11:O:72:PRO:HD3	1.59	0.82
5:F:28:ILE:CD1	5:F:119:ARG:HE	1.91	0.82
3:D:34:VAL:HG21	3:D:35:LYS:HZ3	1.44	0.82
28:6:14:THR:O	28:6:49:HIS:CA	2.28	0.81
7:H:127:GLU:HG2	7:H:128:PRO:HD3	1.57	0.81
1:A:1063:G:O6	1:A:1075:C:N4	2.14	0.81
2:B:5:C:H42	2:B:115:G:H1	1.28	0.81
4:E:69:LYS:H	4:E:69:LYS:HD2	1.43	0.81
1:A:2658:C:N4	1:A:2663:G:O6	2.11	0.81
7:H:149:ARG:HA	7:H:162:ILE:HG21	1.63	0.81
1:A:1652:A:OP1	13:O:8:ARG:NH1	2.13	0.81
4:E:87:GLU:O	4:E:89:ASP:N	2.13	0.81
7:H:3:ARG:HG3	7:H:4:ILE:HG12	1.62	0.81
4:E:23:VAL:HG21	4:E:183:LEU:HG	1.63	0.81
4:E:11:MET:HG3	4:E:24:THR:HG22	1.61	0.81
1:A:1079:C:N4	1:A:1088:A:OP1	2.14	0.80
1:A:1019:U:OP1	1:A:1035:U:O2'	1.99	0.80
1:A:84:A:N6	1:A:102:G:O2'	2.14	0.80
4:E:66:HIS:CD2	4:E:67:PHE:CD1	2.69	0.80
1:A:219:G:N2	1:A:234:C:O2	2.14	0.80
28:6:15:GLU:HG3	28:6:47:THR:HG21	1.61	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2749:A:H4'	7:H:62:LYS:HG2	1.62	0.80
1:A:2542:A:O2'	1:A:2543:G:O5'	1.99	0.80
5:F:26:ALA:O	5:F:27:GLU:CG	2.30	0.80
2:B:30:C:H42	2:B:54:G:H1	1.28	0.80
5:F:63:LYS:NZ	5:F:67:GLN:HE21	1.79	0.80
7:H:6:ARG:HE	7:H:62:LYS:HE3	1.44	0.80
11:O:60:MET:O	11:O:61:ARG:CD	2.30	0.80
1:A:1800:C:OP2	3:D:183:ARG:NH2	2.15	0.80
3:D:35:LYS:CG	3:D:64:ILE:HG23	2.10	0.80
21:V:59:LEU:O	21:V:61:LEU:N	2.14	0.79
7:H:92:ILE:HG22	7:H:93:GLY:H	1.45	0.79
4:E:26:ILE:O	4:E:27:LEU:HB2	1.83	0.79
2:B:86:G:N1	2:B:90:C:N3	2.27	0.79
1:A:2795:G:N7	1:A:2797:U:O2'	2.15	0.79
3:D:35:LYS:HE3	3:D:64:ILE:CG1	2.13	0.79
1:A:2849:U:O4	15:R:23:ARG:NH2	2.14	0.79
3:D:35:LYS:HE3	3:D:64:ILE:C	2.02	0.79
11:O:60:MET:O	11:O:61:ARG:CG	2.30	0.79
1:A:1069:A:H5'	1:A:1070:A:C8	2.18	0.79
1:A:2808:U:O2	1:A:2892:A:N6	2.16	0.79
3:D:25:THR:HG22	3:D:82:ILE:H	1.46	0.79
28:6:19:ARG:HH21	28:6:52:VAL:HG11	1.46	0.79
1:A:1111:A:H1'	7:H:2:SER:HA	1.65	0.79
1:A:886:C:H2'	1:A:888:C:H42	1.46	0.79
6:G:67:LYS:HB3	26:4:6:HIS:HD2	1.46	0.79
4:E:26:ILE:HG22	4:E:27:LEU:N	1.98	0.79
4:E:63:LEU:O	4:E:64:LYS:CG	2.30	0.79
5:F:188:ARG:HA	11:O:3:LEU:HD11	1.65	0.78
1:A:2068:U:H3	1:A:2430:A:H2	1.29	0.78
3:D:35:LYS:HG3	3:D:64:ILE:N	1.97	0.78
11:O:64:LYS:O	11:O:64:LYS:CD	2.32	0.78
28:6:14:THR:CB	28:6:20:ASN:O	2.31	0.78
2:B:80:U:H2'	2:B:81:G:H21	1.48	0.78
1:A:2287:A:H62	1:A:2344:U:H3	1.32	0.78
1:A:654(B):C:O2	1:A:654(S):G:N2	2.12	0.78
30:8:40:GLU:H	30:8:43:GLN:HG3	1.48	0.78
11:O:11:GLY:O	11:O:13:ASN:N	2.17	0.78
2:B:18:G:N2	2:B:65:C:N3	2.30	0.78
12:P:43:THR:HB	12:P:45:GLN:HE21	1.48	0.78
1:A:288:C:N4	1:A:353:G:O6	2.15	0.78
1:A:2746:U:OP1	7:H:85:LYS:NZ	2.14	0.78
1:A:1332:G:N2	1:A:1609:A:O2'	2.16	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1188:U:H4'	17:2:79:VAL:HG11	1.66	0.78
5:F:53:THR:HG23	5:F:55:GLY:H	1.48	0.78
1:A:2137:C:N4	1:A:2154:G:O6	2.18	0.77
2:B:24:G:N3	2:B:27:C:N4	2.32	0.77
3:D:35:LYS:NZ	3:D:64:ILE:HG12	1.99	0.77
1:A:2467:C:H4'	12:P:123:HIS:CD2	2.19	0.77
1:A:2744:G:N2	7:H:143:GLN:OE1	2.18	0.77
1:A:660:G:H21	11:O:12:ALA:HA	1.49	0.77
1:A:1678:G:N2	1:A:1989:G:H22	1.80	0.77
3:D:34:VAL:CG2	3:D:35:LYS:HE2	2.09	0.77
11:O:71:VAL:HG12	11:O:72:PRO:HD3	0.79	0.77
18:S:65:LEU:HD13	18:S:68:ARG:HD2	1.67	0.77
1:A:2666:C:N3	7:H:152:ARG:NH2	2.33	0.77
3:D:35:LYS:HZ1	3:D:64:ILE:HG12	1.50	0.77
1:A:2357:U:OP1	22:3:20:ARG:NH1	2.15	0.77
4:E:67:PHE:HE2	4:E:69:LYS:HZ2	1.29	0.77
5:F:25:PRO:HB3	5:F:119:ARG:HD3	1.65	0.77
21:V:92:SER:O	21:V:94:GLU:N	2.17	0.77
11:O:71:VAL:HG13	11:O:72:PRO:CD	2.14	0.77
1:A:1049:C:N3	7:H:2:SER:N	2.33	0.77
1:A:2343:C:O2'	1:A:2373:G:O2'	1.97	0.77
1:A:1542:G:H3'	1:A:1543:A:H5''	1.67	0.77
5:F:3:GLU:CA	5:F:24:LEU:HG	2.14	0.77
1:A:529:A:H4'	1:A:530:G:H5'	1.67	0.77
1:A:1689:A:H62	1:A:1698:A:H2	1.31	0.77
11:O:62:LEU:CD1	30:8:25:MET:HB2	2.14	0.76
20:U:50:ARG:C	20:U:53:PRO:HD3	2.05	0.76
4:E:9:VAL:CG2	4:E:25:VAL:CG1	2.61	0.76
4:E:66:HIS:CG	4:E:67:PHE:HA	2.20	0.76
4:E:63:LEU:O	4:E:64:LYS:CB	2.32	0.76
6:G:68:PRO:HA	6:G:92:VAL:HB	1.66	0.76
21:V:151:HIS:HB3	21:V:167:PRO:HB3	1.67	0.76
3:D:34:VAL:HG23	3:D:35:LYS:HZ3	1.07	0.76
28:6:15:GLU:CG	28:6:16:CYS:H	1.91	0.76
1:A:993:G:OP1	16:1:50:ARG:NH2	2.17	0.76
15:R:55:ASN:H	15:R:59:THR:HG22	1.50	0.76
1:A:2873:A:H8	13:0:6:SER:H	1.33	0.76
21:V:77:ASP:OD2	21:V:80:ARG:NH1	2.19	0.76
1:A:2297:C:O2	1:A:2321:G:N2	2.15	0.76
9:M:4:TYR:O	16:1:64:ARG:NH1	2.18	0.76
9:M:56:ASN:H	9:M:125:GLY:HA3	1.51	0.76
5:F:66:PRO:O	5:F:67:GLN:CB	2.32	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
21:V:161:VAL:HG23	21:V:162:GLU:HG2	1.67	0.76
12:P:26:TYR:OH	12:P:141:GLN:OE1	2.03	0.76
17:2:10:LYS:NZ	17:2:23:GLU:OE1	2.15	0.76
5:F:8:GLN:HA	5:F:15:SER:HA	1.68	0.76
28:6:14:THR:O	28:6:49:HIS:CB	2.33	0.76
1:A:2638:G:P	4:E:82:ARG:NH2	2.55	0.76
21:V:103:ARG:HB2	21:V:138:GLU:HA	1.66	0.76
3:D:17:THR:O	3:D:211:ARG:NH2	2.19	0.76
1:A:1093:G:N1	1:A:1097:U:OP2	2.19	0.75
14:Q:3:ARG:HE	14:Q:4:LEU:N	1.83	0.75
4:E:11:MET:CE	4:E:24:THR:CG2	2.64	0.75
1:A:1728:G:H8	1:A:1732:A:H62	1.33	0.75
30:8:29:LYS:HB2	30:8:44:LYS:HB3	1.67	0.75
26:4:39:CYS:HB3	26:4:41:PRO:CD	2.17	0.75
1:A:93:C:C5'	20:U:54:LYS:NZ	2.50	0.75
1:A:1036:G:N1	1:A:1119:C:N3	2.29	0.75
11:O:62:LEU:HD22	30:8:27:THR:CG2	2.17	0.75
1:A:1899:G:H21	1:A:1902:C:N4	1.84	0.75
1:A:1036:G:N2	1:A:1119:C:O2	2.15	0.75
11:O:62:LEU:N	11:O:63:PRO:HD3	1.96	0.75
2:B:86:G:O6	2:B:90:C:N4	2.15	0.75
4:E:13:ARG:CA	4:E:21:VAL:O	2.35	0.74
11:O:60:MET:C	11:O:61:ARG:HG2	2.06	0.74
2:B:1(M):A:N6	2:B:117:G:N7	2.35	0.74
1:A:2420:C:H41	30:8:31:HIS:HB3	1.52	0.74
14:Q:12:PHE:O	14:Q:16:ASN:ND2	2.20	0.74
16:1:90:VAL:O	16:1:92:ARG:N	2.21	0.74
4:E:69:LYS:N	4:E:69:LYS:HD2	2.03	0.74
18:S:59:VAL:HG23	18:S:65:LEU:H	1.51	0.74
26:4:56:VAL:HA	26:4:60:GLN:HE22	1.50	0.74
5:F:101:LEU:O	5:F:106:ARG:NH1	2.20	0.74
1:A:527:C:N4	1:A:2779:U:OP2	2.21	0.74
9:M:91:LEU:HA	9:M:95:PRO:HB3	1.68	0.74
1:A:780:G:H21	1:A:783:A:H62	1.35	0.74
2:B:15:A:H5'	2:B:16:G:C8	2.21	0.74
1:A:2139:C:H42	1:A:2152:G:H1	1.36	0.74
1:A:1171:G:O2'	1:A:1173:G:O5'	2.04	0.74
1:A:93:C:H4'	20:U:54:LYS:NZ	2.03	0.74
1:A:774:A:H2	1:A:787:U:HO2'	1.35	0.74
1:A:854:G:O6	1:A:923:C:N4	2.20	0.74
1:A:403:U:H4'	1:A:404:C:H5'	1.70	0.74
1:A:1037:G:O6	1:A:1118:C:N4	2.17	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1477:A:N6	1:A:1516:U:O4	2.18	0.74
1:A:989:G:OP2	25:X:11:SER:OG	2.05	0.73
1:A:2652:C:H42	1:A:2668:G:H1	1.36	0.73
1:A:768:G:O2'	1:A:1379:A:N6	2.21	0.73
1:A:1039:G:O6	1:A:1116:C:N4	2.19	0.73
1:A:2124:G:O6	1:A:2174:C:N4	2.16	0.73
1:A:2875:C:H4'	15:R:5:ALA:HB2	1.69	0.73
11:O:62:LEU:HD11	30:8:25:MET:CA	2.16	0.73
1:A:889:C:H2'	1:A:890:A:H4'	1.70	0.73
5:F:25:PRO:O	5:F:26:ALA:HB3	1.89	0.73
4:E:69:LYS:O	4:E:70:ALA:HB2	1.88	0.73
5:F:25:PRO:O	5:F:26:ALA:CB	2.36	0.73
26:4:39:CYS:C	26:4:40:HIS:ND1	2.42	0.73
1:A:2757:A:N1	7:H:67:LEU:HD11	2.03	0.73
10:N:63:VAL:HG12	10:N:106:LEU:HD11	1.71	0.73
1:A:1070:A:H8	1:A:1096:A:H1'	1.52	0.73
1:A:2749:A:N1	1:A:2750:A:N6	2.36	0.73
28:6:14:THR:HG21	28:6:19:ARG:HG3	1.69	0.73
28:6:12:GLU:HG3	28:6:21:TYR:CE1	2.23	0.73
1:A:2365:G:N7	30:8:39:LYS:NZ	2.36	0.73
13:0:34:ILE:HG22	13:0:114:VAL:HB	1.69	0.73
1:A:2681:C:H5	1:A:2725:A:H62	1.36	0.73
5:F:28:ILE:HD13	5:F:119:ARG:HH21	1.53	0.72
1:A:1057:A:N6	1:A:1088:A:OP2	2.21	0.72
13:0:67:LEU:HD12	13:0:76:VAL:HG21	1.71	0.72
24:W:22:GLU:HG2	24:W:64:LEU:HD11	1.71	0.72
2:B:49:C:OP2	14:Q:30:ARG:NH1	2.23	0.72
1:A:1105:U:H2'	1:A:1106:G:H8	1.53	0.72
1:A:1247:A:OP1	5:F:95:ARG:NH2	2.22	0.72
10:N:120:GLU:OE2	15:R:67:SER:OG	2.07	0.72
1:A:7:G:H1	1:A:2896:C:H42	1.38	0.72
11:O:47:ASP:HB3	11:O:48:PRO:HA	1.72	0.72
1:A:883:G:H1	1:A:893:C:N4	1.87	0.72
1:A:661:C:O2'	11:O:13:ASN:O	2.06	0.72
1:A:1225:C:O2'	17:2:85:LYS:N	2.15	0.72
16:1:90:VAL:HG22	17:2:39:LEU:HB3	1.71	0.71
1:A:1071:G:N3	1:A:1089:G:O2'	2.22	0.71
1:A:1093:G:H22	1:A:1097:U:H5''	1.54	0.71
1:A:2163:C:H5''	1:A:2171:A:C8	2.25	0.71
6:G:11:TYR:HA	6:G:15:VAL:HB	1.73	0.71
1:A:2023:G:OP2	1:A:2617:C:H4'	1.90	0.71
1:A:2611:U:H2'	27:5:3:LYS:HG3	1.72	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:F:133:ASN:ND2	5:F:138:GLU:OE2	2.23	0.71
30:8:33:ASN:HA	30:8:34:TRP:CE3	2.26	0.71
3:D:85:ASP:HB2	3:D:92:ILE:HD13	1.72	0.71
1:A:2:G:H1	1:A:2901:C:H42	1.38	0.71
21:V:33:LEU:HD23	21:V:90:VAL:HG21	1.73	0.71
1:A:1228:G:OP2	16:1:16:LYS:NZ	2.22	0.71
1:A:1569:A:H2'	1:A:1570:A:C8	2.26	0.71
7:H:6:ARG:NE	7:H:62:LYS:HE3	2.05	0.71
4:E:76:ARG:O	4:E:78:LEU:N	2.22	0.71
26:4:43:TYR:O	26:4:46:GLN:N	2.23	0.71
1:A:907:U:O2'	12:P:101:ARG:NH2	2.21	0.71
4:E:60:ASN:ND2	4:E:63:LEU:HD21	2.03	0.71
4:E:72:VAL:HG12	4:E:72:VAL:O	1.90	0.71
1:A:2315:G:OP1	6:G:36:LYS:NZ	2.22	0.71
6:G:36:LYS:HE2	6:G:160:VAL:HG21	1.72	0.71
1:A:958:U:OP2	12:P:14:ARG:NH1	2.23	0.71
11:O:62:LEU:N	11:O:63:PRO:CD	2.52	0.70
1:A:1058:U:H2'	1:A:1059:G:C8	2.26	0.70
4:E:9:VAL:HG21	4:E:25:VAL:HG11	1.72	0.70
16:1:92:ARG:HG3	16:1:94:ASN:HB3	1.73	0.70
21:V:157:LEU:HB3	21:V:161:VAL:HG12	1.71	0.70
21:V:10:ARG:NH2	21:V:26:GLY:O	2.25	0.70
1:A:1012:U:H3	1:A:1143:A:H2	1.37	0.70
14:Q:35:ILE:HD11	14:Q:97:ARG:HE	1.57	0.70
4:E:11:MET:HE3	4:E:24:THR:CG2	2.22	0.70
11:O:62:LEU:HD22	30:8:27:THR:HG23	1.73	0.70
28:6:47:THR:HG23	28:6:47:THR:O	1.89	0.70
1:A:2343:C:HO2'	1:A:2373:G:HO2'	1.21	0.70
1:A:2471:C:N4	1:A:2476:A:O2'	2.24	0.70
2:B:57:A:H1'	6:G:29:TRP:HB2	1.74	0.70
17:2:35:LEU:HG	17:2:37:VAL:HG13	1.72	0.70
17:2:47:VAL:O	17:2:47:VAL:CG2	2.40	0.70
3:D:30:GLU:OE1	3:D:63:ARG:NE	2.22	0.70
17:2:34:GLU:OE1	17:2:56:SER:OG	2.10	0.69
1:A:602:G:HO2'	1:A:604:G:HO2'	1.32	0.69
1:A:443:A:N6	5:F:41:LEU:O	2.25	0.69
1:A:270(H):C:O2	23:Z:78:LYS:NZ	2.24	0.69
4:E:71:GLY:C	4:E:73:GLU:H	1.95	0.69
1:A:1225:C:HO2'	17:2:85:LYS:H	1.37	0.69
17:2:69:LYS:HD2	17:2:86:GLY:HA3	1.73	0.69
11:O:64:LYS:HD2	30:8:25:MET:SD	2.32	0.69
1:A:2134:A:N6	1:A:2157:G:O2'	2.24	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:G:105:LYS:HG2	26:4:24:THR:HG22	1.73	0.69
26:4:23:GLU:O	26:4:25:TYR:N	2.24	0.69
1:A:2318:G:H22	14:Q:3:ARG:HB2	1.56	0.69
20:U:49:VAL:O	20:U:51:VAL:N	2.25	0.69
4:E:26:ILE:O	4:E:27:LEU:CB	2.41	0.69
17:2:91:TYR:O	17:2:91:TYR:HD2	1.75	0.69
1:A:1141:U:OP2	9:M:63:THR:OG1	2.10	0.69
23:Z:92:LYS:O	23:Z:94:LEU:N	2.24	0.69
2:B:28:C:H42	2:B:56:G:H1	1.38	0.69
2:B:48:A:H4'	14:Q:95:HIS:HD2	1.58	0.69
1:A:1105:U:H2'	1:A:1106:G:C8	2.28	0.69
6:G:67:LYS:HB3	26:4:6:HIS:CD2	2.28	0.69
1:A:1332:G:H21	1:A:1610:A:H8	1.40	0.69
3:D:35:LYS:CE	3:D:64:ILE:HG23	2.22	0.69
1:A:1141:U:OP1	9:M:25:ARG:NH1	2.21	0.69
27:5:16:ARG:NH1	27:5:17:ASP:OD1	2.25	0.69
10:N:88:ASN:HB3	10:N:94:ARG:HD3	1.74	0.69
1:A:2438:U:O3'	1:A:2439:A:H3'	1.93	0.69
20:U:42:VAL:HG13	20:U:65:ALA:HB3	1.74	0.69
4:E:105:THR:OG1	4:E:199:ARG:NH2	2.25	0.69
1:A:1077:A:O2'	1:A:1078:U:O4'	2.09	0.69
11:O:52:GLU:OE1	11:O:54:GLY:N	2.26	0.68
1:A:2120:G:H1	1:A:2178:C:H42	1.41	0.68
1:A:2162:G:H2'	1:A:2163:C:H6	1.58	0.68
26:4:16:CYS:H	26:4:20:ASN:H	1.41	0.68
3:D:148:GLU:HB2	3:D:151:LYS:HD2	1.75	0.68
7:H:30:LYS:NZ	7:H:79:VAL:O	2.26	0.68
4:E:26:ILE:HG22	4:E:27:LEU:H	1.57	0.68
14:Q:26:LEU:HD22	14:Q:87:PHE:HD1	1.58	0.68
1:A:2173:A:N6	1:A:2174:C:HO2'	1.92	0.68
4:E:36:ARG:NH1	4:E:85:ASN:OD1	2.26	0.68
21:V:70:LEU:HD11	21:V:98:MET:HE3	1.75	0.68
6:G:94:LEU:HD12	6:G:99:MET:HA	1.76	0.68
21:V:132:ASN:HD22	21:V:159:PRO:HB2	1.58	0.68
1:A:561:G:H1'	16:1:45:TYR:HE1	1.58	0.68
1:A:873:G:H1	1:A:904:C:H42	1.39	0.68
4:E:12:THR:O	4:E:22:PRO:HA	1.93	0.68
22:3:18:ALA:HB3	22:3:20:ARG:HH21	1.58	0.68
15:R:125:ARG:NH1	15:R:128:GLU:OE2	2.26	0.68
15:R:64:ARG:HB2	15:R:73:GLU:HG2	1.76	0.68
4:E:11:MET:HG3	4:E:24:THR:CG2	2.23	0.68
5:F:63:LYS:HZ1	5:F:67:GLN:HE21	1.43	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
22:3:27:GLU:HB2	22:3:69:PHE:HD2	1.59	0.68
21:V:10:ARG:HH21	21:V:26:GLY:H	1.42	0.68
17:2:37:VAL:O	17:2:51:VAL:CG1	2.42	0.67
5:F:102:PRO:HB2	5:F:105:VAL:HG23	1.76	0.67
11:O:21:ARG:HE	11:O:21:ARG:HA	1.57	0.67
26:4:39:CYS:O	26:4:40:HIS:CB	2.43	0.67
19:T:90:GLU:HA	19:T:93:GLU:HB2	1.75	0.67
3:D:35:LYS:CD	3:D:64:ILE:CG2	2.49	0.67
28:6:15:GLU:CG	28:6:47:THR:HG21	2.23	0.67
4:E:67:PHE:HE2	4:E:69:LYS:NZ	1.93	0.67
1:A:300:A:OP2	20:U:84:ARG:NH1	2.23	0.67
1:A:1725:G:N1	1:A:1735:C:N3	2.34	0.67
3:D:35:LYS:HE2	3:D:64:ILE:O	1.94	0.67
5:F:23:ASP:C	5:F:24:LEU:HD22	2.15	0.67
1:A:1022:G:O2'	1:A:1023:U:OP2	2.11	0.67
11:O:47:ASP:OD2	11:O:50:ARG:NH1	2.28	0.67
21:V:146:ILE:HD12	21:V:147:GLY:N	2.04	0.67
1:A:2135:A:H62	1:A:2156:G:H21	1.43	0.67
4:E:4:ILE:HD11	4:E:28:ALA:HB1	1.77	0.67
16:1:66:ASN:HD21	16:1:70:ARG:HE	1.43	0.67
1:A:390:A:C6	11:O:71:VAL:HG21	2.30	0.67
4:E:66:HIS:CD2	4:E:67:PHE:HA	2.30	0.67
1:A:1084:A:N7	1:A:1085:A:N6	2.42	0.67
1:A:675:A:N3	1:A:2443:C:O2'	2.28	0.67
26:4:39:CYS:O	26:4:41:PRO:HD3	1.95	0.66
1:A:2183:C:H2'	1:A:2184:G:H8	1.59	0.66
1:A:1141:U:P	9:M:25:ARG:HH12	2.18	0.66
11:O:85:LEU:HA	11:O:88:LEU:HB3	1.77	0.66
17:2:52:VAL:CG1	17:2:55:ALA:HB3	2.25	0.66
2:B:56:G:H5'	6:G:27:ASN:HD22	1.59	0.66
9:M:42:TRP:O	16:1:64:ARG:NH2	2.28	0.66
1:A:1414:G:O6	1:A:1587:A:N6	2.28	0.66
2:B:114:G:O2'	14:Q:50:SER:OG	2.13	0.66
1:A:288:C:N3	1:A:353:G:N1	2.34	0.66
17:2:37:VAL:O	17:2:51:VAL:HG11	1.95	0.66
11:O:13:ASN:O	11:O:15:ARG:N	2.26	0.66
1:A:2313:C:H4'	6:G:91:ARG:HG3	1.77	0.66
3:D:246:PRO:HD2	3:D:255:LYS:HG2	1.76	0.66
4:E:63:LEU:O	4:E:64:LYS:HB2	1.95	0.66
1:A:1725:G:O6	1:A:1735:C:N4	2.16	0.66
1:A:1184:G:OP2	25:X:30:ARG:NH2	2.29	0.66
1:A:1011:G:N2	1:A:1150:C:N3	2.41	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:F:28:ILE:HD12	5:F:119:ARG:HE	1.61	0.66
5:F:24:LEU:HD22	5:F:24:LEU:N	2.11	0.66
5:F:63:LYS:HE2	5:F:67:GLN:HB2	1.77	0.66
28:6:14:THR:HB	28:6:20:ASN:C	2.17	0.66
5:F:132:VAL:HG22	5:F:133:ASN:H	1.61	0.66
6:G:145:THR:O	6:G:147:ASP:N	2.28	0.66
1:A:2816:C:O3'	13:0:99:LYS:NZ	2.28	0.66
3:D:31:LYS:NZ	3:D:94:LEU:HD11	2.10	0.65
11:O:121:LYS:HB3	11:O:123:LEU:HD22	1.76	0.65
16:1:72:HIS:HD2	16:1:110:VAL:HG21	1.59	0.65
1:A:908:C:O2'	12:P:71:ASP:OD2	2.12	0.65
4:E:67:PHE:CE2	4:E:69:LYS:NZ	2.64	0.65
4:E:60:ASN:CB	4:E:63:LEU:HD11	2.21	0.65
1:A:2130:U:H2'	1:A:2158:A:N1	2.10	0.65
7:H:20:ALA:HB3	7:H:23:ARG:HB2	1.78	0.65
21:V:76:LEU:HA	21:V:83:PRO:HA	1.77	0.65
1:A:2134:A:H62	1:A:2158:A:H8	1.45	0.65
7:H:6:ARG:HB2	7:H:6:ARG:HH11	1.60	0.65
8:K:143:SER:OG	8:K:144:VAL:N	2.25	0.65
2:B:56:G:H5'	6:G:27:ASN:ND2	2.11	0.65
1:A:1332:G:N2	1:A:1609:A:HO2'	1.94	0.65
1:A:1225:C:O2	17:2:84:LYS:NZ	2.27	0.65
9:M:103:VAL:HG11	9:M:120:LEU:HD13	1.79	0.65
1:A:1359:A:H62	1:A:1372:U:H3	1.43	0.65
15:R:93:ARG:HG2	15:R:117:ASP:HB3	1.79	0.65
1:A:2133:G:H2'	1:A:2157:G:H1	1.62	0.65
26:4:13:ARG:HG2	26:4:22:ILE:HG23	1.79	0.65
5:F:132:VAL:O	5:F:134:GLY:N	2.24	0.65
1:A:2210:G:H3'	1:A:2211:G:C5	2.31	0.65
4:E:71:GLY:O	4:E:73:GLU:N	2.30	0.65
1:A:2290:G:H1	1:A:2342:C:H42	1.44	0.65
1:A:2817:G:P	13:0:99:LYS:HZ3	2.20	0.65
7:H:89:ILE:HD12	7:H:129:THR:HB	1.79	0.65
6:G:120:LEU:HB2	6:G:180:PHE:HD1	1.61	0.65
1:A:2287:A:N6	1:A:2344:U:H3	1.93	0.65
11:O:49:ARG:CG	11:O:49:ARG:O	2.30	0.65
26:4:39:CYS:O	26:4:40:HIS:HB2	1.96	0.65
7:H:86:GLU:HG3	7:H:132:ARG:HB3	1.77	0.65
9:M:15:LEU:HD23	9:M:134:ARG:HG3	1.79	0.65
1:A:1467:C:H42	1:A:1525:G:H1	1.44	0.65
1:A:1434:A:H61	1:A:1558:A:H62	1.44	0.65
26:4:40:HIS:N	26:4:41:PRO:HD2	2.11	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:33:G:OP2	6:G:96:ARG:NH2	2.30	0.64
15:R:26:ASP:OD1	15:R:120:ARG:NH2	2.27	0.64
18:S:88:ARG:NH1	18:S:94:ASP:OD2	2.24	0.64
7:H:7:LEU:HD12	7:H:8:PRO:HD3	1.79	0.64
3:D:31:LYS:HE3	3:D:33:LEU:HD12	1.79	0.64
1:A:2485:G:H5''	12:P:46:GLN:HE21	1.62	0.64
1:A:1899:G:N2	1:A:1902:C:H41	1.95	0.64
1:A:2059:A:H5'	1:A:2060:A:OP2	1.96	0.64
17:2:62:LEU:HD11	17:2:95:LEU:HD12	1.80	0.64
1:A:1300:U:H4'	1:A:1301:A:H5'	1.78	0.64
4:E:131:ALA:HB1	4:E:135:HIS:CE1	2.33	0.64
4:E:11:MET:CG	4:E:24:THR:CG2	2.63	0.64
1:A:2392:A:H2	1:A:2424:C:H42	1.43	0.64
1:A:2415:G:O3'	11:O:66:GLY:HA3	1.97	0.64
14:Q:19:LYS:O	14:Q:21:THR:N	2.31	0.64
17:2:68:LYS:HD2	17:2:69:LYS:H	1.62	0.64
15:R:3:ARG:HG2	15:R:6:LEU:HB2	1.79	0.64
1:A:859:G:O2'	1:A:916:G:O6	2.15	0.64
17:2:49:THR:O	17:2:50:PRO:C	2.36	0.64
2:B:44:G:OP1	6:G:98:ARG:NH2	2.30	0.64
1:A:1394:U:O2	19:T:16:LYS:NZ	2.29	0.64
28:6:14:THR:OG1	28:6:15:GLU:N	2.30	0.64
4:E:63:LEU:HB3	4:E:73:GLU:OE1	1.98	0.64
1:A:2469:A:O2'	12:P:56:ARG:NE	2.31	0.64
17:2:32:THR:HG22	17:2:60:GLU:HB3	1.79	0.64
14:Q:88:ASP:OD1	14:Q:90:GLY:N	2.19	0.64
15:R:107:ASP:N	15:R:107:ASP:OD1	2.29	0.64
5:F:107:LYS:NZ	5:F:205:ARG:O	2.30	0.64
20:U:55:TYR:O	20:U:56:PRO:C	2.36	0.64
1:A:34:C:O2'	1:A:35:G:OP2	2.14	0.64
17:2:1:MET:HG3	17:2:43:GLU:H	1.63	0.64
7:H:129:THR:OG1	7:H:130:ARG:N	2.27	0.64
4:E:10:GLY:O	4:E:24:THR:O	2.16	0.63
3:D:69:ARG:O	3:D:71:ASP:N	2.31	0.63
28:6:17:LYS:O	28:6:19:ARG:N	2.30	0.63
6:G:112:PRO:HB2	26:4:35:VAL:HG11	1.80	0.63
1:A:523:C:O2	1:A:553:U:O2'	2.15	0.63
1:A:39:C:O2	5:F:46:ARG:NH2	2.32	0.63
1:A:1007:C:OP1	9:M:35:ARG:NH1	2.30	0.63
1:A:851:U:OP1	25:X:49:LYS:NZ	2.26	0.63
11:O:60:MET:C	11:O:61:ARG:CG	2.66	0.63
24:W:42:GLY:O	24:W:44:LEU:N	2.28	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:995:C:O2	9:M:3:THR:OG1	2.16	0.63
7:H:33:LEU:HD12	7:H:75:ALA:HA	1.79	0.63
4:E:23:VAL:CG2	4:E:183:LEU:HG	2.26	0.63
3:D:35:LYS:HG3	3:D:64:ILE:H	1.61	0.63
11:O:61:ARG:O	11:O:62:LEU:CB	2.32	0.63
9:M:24:GLY:O	9:M:28:THR:HG22	1.99	0.63
1:A:1593:G:H2'	1:A:1594:G:C8	2.34	0.63
28:6:47:THR:O	28:6:48:VAL:O	2.16	0.63
1:A:1817:G:OP1	3:D:88:ARG:NH2	2.30	0.63
14:Q:23:ARG:NH2	14:Q:84:GLN:OE1	2.31	0.63
1:A:892:G:N7	1:A:893:C:N4	2.46	0.63
1:A:1075:C:OP2	1:A:1077:A:N6	2.32	0.63
1:A:389:G:H22	11:O:71:VAL:HG12	1.63	0.63
28:6:15:GLU:CG	28:6:47:THR:CG2	2.75	0.63
7:H:81:GLU:HG2	7:H:83:TYR:HB2	1.80	0.63
6:G:67:LYS:H	26:4:6:HIS:CD2	2.17	0.63
1:A:2415:G:H4'	11:O:67:MET:N	2.13	0.63
14:Q:15:ARG:HH12	14:Q:90:GLY:HA2	1.63	0.63
20:U:88:LYS:O	20:U:90:LEU:N	2.32	0.63
15:R:36:GLU:OE1	15:R:41:ARG:NH1	2.32	0.63
1:A:635:C:O2'	1:A:639:U:OP1	2.17	0.63
11:O:52:GLU:OE1	11:O:55:ARG:N	2.21	0.63
7:H:4:ILE:HG21	7:H:6:ARG:NH2	2.13	0.63
12:P:19:GLY:H	12:P:98:LYS:NZ	1.95	0.63
1:A:1266:G:O5'	18:S:15:ARG:NH2	2.32	0.63
4:E:120:TRP:CD1	4:E:155:LYS:HB3	2.33	0.63
1:A:2306:C:N4	6:G:42:GLY:O	2.31	0.63
25:X:3:ARG:NH1	25:X:38:GLU:OE2	2.32	0.63
1:A:1062:G:N2	1:A:1076:C:H42	1.96	0.62
14:Q:109:GLY:O	14:Q:111:GLU:N	2.32	0.62
21:V:100:VAL:HG11	21:V:134:PRO:HG2	1.81	0.62
1:A:96:G:H4'	24:W:48:HIS:CD2	2.34	0.62
11:O:125:VAL:HG13	11:O:144:GLU:HB3	1.81	0.62
7:H:158:HIS:ND1	7:H:158:HIS:O	2.32	0.62
21:V:129:SER:OG	21:V:132:ASN:OD1	2.17	0.62
1:A:326:G:H1	1:A:336:C:H42	1.46	0.62
4:E:51:PHE:O	4:E:74:PRO:HB2	1.99	0.62
6:G:108:ASN:HB3	26:4:38:LYS:CD	2.29	0.62
1:A:1093:G:H1	1:A:1097:U:P	2.22	0.62
1:A:2658:C:N3	1:A:2663:G:N1	2.34	0.62
1:A:1542:G:O6	1:A:1543:A:N6	2.32	0.62
1:A:1534:G:H2'	1:A:1537:C:H42	1.63	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:N:68:GLU:HB3	10:N:78:ARG:NH1	2.15	0.62
26:4:43:TYR:O	26:4:45:GLY:N	2.32	0.62
1:A:1061:U:H4'	1:A:1070:A:H1'	1.81	0.62
1:A:2135:A:N3	1:A:2159:G:O2'	2.32	0.62
1:A:1064:C:H2'	1:A:1065:U:H5	1.64	0.62
1:A:1568:G:OP2	3:D:63:ARG:NH2	2.30	0.62
11:O:30:THR:HG21	11:O:35:HIS:H	1.64	0.62
1:A:2126:A:N6	1:A:2163:C:O2	2.31	0.62
4:E:47:VAL:HG22	4:E:48:GLN:H	1.63	0.62
21:V:29:TYR:HE1	21:V:87:ASP:HB3	1.64	0.62
1:A:1464:C:HO2'	1:A:1528:A:H8	1.45	0.62
4:E:101:ARG:NH1	4:E:171:GLU:HB2	2.13	0.62
5:F:63:LYS:NZ	5:F:67:GLN:NE2	2.46	0.62
1:A:783:A:H8	1:A:784:A:H4'	1.64	0.62
3:D:63:ARG:H	3:D:87:ASN:HD21	1.48	0.62
1:A:1183:G:O3'	25:X:29:ARG:NH2	2.33	0.62
11:O:60:MET:O	11:O:61:ARG:CB	2.48	0.62
4:E:18:ASP:HB3	15:R:82:LEU:HD11	1.80	0.62
1:A:153:C:OP2	23:Z:88:LYS:NZ	2.20	0.62
5:F:143:ALA:HB1	5:F:148:LEU:HB2	1.80	0.62
3:D:146:GLU:HB2	3:D:189:CYS:HB3	1.81	0.62
27:5:45:VAL:HG13	27:5:50:GLY:HA2	1.80	0.62
17:2:2:PHE:H	17:2:42:GLY:HA3	1.65	0.62
17:2:45:THR:O	17:2:47:VAL:HG12	1.99	0.62
1:A:1139:G:HO2'	1:A:1143:A:H62	1.48	0.62
14:Q:26:LEU:HB3	14:Q:87:PHE:HA	1.82	0.62
4:E:28:ALA:HB3	4:E:93:VAL:HG22	1.82	0.62
1:A:2191:G:O2'	1:A:2192:G:OP1	2.15	0.62
5:F:2:LYS:C	5:F:24:LEU:HG	2.19	0.61
2:B:38:C:O4'	14:Q:95:HIS:NE2	2.32	0.61
1:A:1138:G:H21	9:M:106:MET:HE3	1.65	0.61
1:A:1309:G:HO2'	1:A:1611:C:HO2'	1.46	0.61
1:A:2228:G:OP1	3:D:261:LYS:NZ	2.25	0.61
1:A:1203:G:H3'	1:A:1204:A:H5''	1.82	0.61
28:6:35:GLU:O	28:6:37:ARG:NH1	2.34	0.61
1:A:883:G:H1	1:A:893:C:H42	1.46	0.61
1:A:2297:C:N3	1:A:2321:G:N1	2.36	0.61
1:A:2415:G:H4'	11:O:67:MET:H	1.65	0.61
8:K:75:LEU:HD13	8:K:139:GLN:HB3	1.83	0.61
6:G:64:THR:HG23	6:G:66:GLN:H	1.64	0.61
26:4:41:PRO:O	26:4:42:PHE:CB	2.49	0.61
8:K:123:LEU:HD22	8:K:143:SER:HA	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:848:G:H2'	1:A:849:A:C8	2.35	0.61
17:2:52:VAL:HG11	17:2:55:ALA:HB3	1.83	0.61
1:A:1771:C:H1'	1:A:1786:A:C8	2.36	0.61
1:A:2602:A:H4'	1:A:2603:G:O5'	1.99	0.61
1:A:69:C:O2	1:A:73:A:O2'	2.17	0.61
26:4:42:PHE:HD1	26:4:43:TYR:N	1.99	0.61
1:A:328:U:H4'	20:U:68:HIS:CE1	2.36	0.61
1:A:2392:A:H1'	11:O:61:ARG:NH2	2.16	0.61
20:U:52:SER:N	20:U:53:PRO:CD	2.63	0.61
2:B:48:A:OP2	14:Q:30:ARG:NH2	2.33	0.61
2:B:104:A:O2'	21:V:30:ASN:O	2.18	0.61
5:F:21:ALA:O	5:F:24:LEU:CD2	2.42	0.61
1:A:1568:G:P	3:D:63:ARG:HH22	2.23	0.61
19:T:55:ASN:HB2	19:T:80:ILE:HG12	1.81	0.61
1:A:2172:U:O2'	1:A:2174:C:OP2	2.14	0.61
1:A:586:A:H5'	5:F:89:VAL:HG21	1.82	0.61
1:A:2119:A:N7	1:A:2170:A:N6	2.49	0.61
6:G:39:ILE:HB	6:G:92:VAL:HG13	1.83	0.61
1:A:2212:A:H1'	1:A:2215:G:C5	2.35	0.61
1:A:654(O):G:H2'	1:A:654(P):G:H8	1.66	0.61
1:A:729:G:OP2	3:D:13:ARG:NH1	2.34	0.61
22:3:27:GLU:HG3	22:3:68:GLU:HA	1.83	0.60
1:A:2839:G:H5'	13:0:46:GLY:HA2	1.81	0.60
1:A:1488:G:H5'	1:A:1489:U:OP2	2.00	0.60
1:A:2748:A:H1'	7:H:67:LEU:HG	1.83	0.60
1:A:1171:G:H1'	1:A:1173:G:OP1	2.00	0.60
1:A:517:C:OP1	27:5:16:ARG:NH2	2.34	0.60
21:V:17:ALA:HA	21:V:20:ARG:HD2	1.82	0.60
4:E:55:ASN:O	4:E:57:LYS:NZ	2.26	0.60
1:A:1071:G:H1'	1:A:1089:G:H2'	1.83	0.60
6:G:11:TYR:OH	6:G:16:ARG:NH2	2.33	0.60
6:G:145:THR:O	6:G:145:THR:OG1	2.14	0.60
6:G:120:LEU:HB2	6:G:180:PHE:CD1	2.36	0.60
4:E:69:LYS:O	4:E:70:ALA:CB	2.49	0.60
1:A:1418:G:OP1	1:A:1588:C:O2'	2.19	0.60
1:A:643:A:N1	1:A:2369:A:O2'	2.32	0.60
20:U:39:VAL:HG23	20:U:41:GLY:H	1.66	0.60
26:4:39:CYS:O	26:4:40:HIS:ND1	2.35	0.60
7:H:6:ARG:NH1	7:H:54:ARG:HH12	2.00	0.60
15:R:1:MET:O	15:R:3:ARG:N	2.34	0.60
1:A:141:A:H8	1:A:1595:G:H21	1.48	0.60
1:A:94:G:H2'	1:A:95:G:O4'	2.02	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:E:35:GLN:HE21	4:E:36:ARG:H	1.48	0.60
1:A:2655:G:N2	1:A:2665:A:OP2	2.35	0.60
21:V:10:ARG:NH2	21:V:26:GLY:H	2.00	0.60
13:0:78:LYS:HE2	13:0:83:ILE:HD11	1.83	0.60
6:G:37:VAL:HG22	6:G:159:VAL:HG12	1.82	0.60
4:E:23:VAL:C	4:E:25:VAL:H	2.04	0.60
1:A:1064:C:H2'	1:A:1065:U:C5	2.36	0.60
21:V:11:GLU:O	21:V:36:LYS:NZ	2.29	0.60
1:A:296:C:H2'	1:A:297:C:H6	1.66	0.60
10:N:4:PRO:O	10:N:5:GLN:HB2	2.00	0.60
28:6:15:GLU:CB	28:6:47:THR:HG23	2.31	0.60
1:A:2542:A:O2'	1:A:2543:G:H8	1.84	0.60
2:B:8:U:OP1	14:Q:11:LYS:NZ	2.33	0.60
1:A:1454:U:O2	13:0:60:LEU:HD11	2.02	0.60
1:A:2131:G:O4'	1:A:2158:A:N6	2.34	0.60
1:A:1055:G:N2	1:A:1104:C:N3	2.50	0.60
20:U:74:PRO:O	20:U:80:GLY:HA2	2.01	0.60
17:2:49:THR:O	17:2:51:VAL:N	2.35	0.60
3:D:34:VAL:CA	3:D:35:LYS:HD3	2.31	0.60
1:A:2365:G:H4'	22:3:60:PHE:CZ	2.37	0.60
2:B:12:C:O2	22:3:74:ARG:NH1	2.35	0.60
1:A:274:G:O2'	1:A:275:G:O4'	2.20	0.60
1:A:2199:A:OP1	23:Z:50:ARG:NH2	2.35	0.60
11:O:63:PRO:HB3	30:8:13:ARG:HG2	1.83	0.59
28:6:43:CYS:O	28:6:44:ARG:C	2.39	0.59
26:4:39:CYS:CB	26:4:41:PRO:CD	2.80	0.59
5:F:160:ASN:OD1	5:F:163:VAL:N	2.33	0.59
6:G:161:THR:HG22	6:G:163:ALA:H	1.66	0.59
1:A:2130:U:O2'	1:A:2133:G:O2'	2.00	0.59
2:B:51:G:N7	14:Q:62:LYS:NZ	2.45	0.59
24:W:41:ILE:HD11	24:W:44:LEU:HD22	1.84	0.59
1:A:1671:U:HO2'	1:A:1673:U:H5	1.50	0.59
11:O:62:LEU:CD1	30:8:25:MET:CB	2.80	0.59
1:A:2287:A:O2'	1:A:2288:A:H5''	2.01	0.59
1:A:960:A:H61	12:P:83:MET:CE	2.14	0.59
19:T:43:VAL:HG23	19:T:51:VAL:HG21	1.84	0.59
1:A:330:A:H2	1:A:1210:A:O2'	1.81	0.59
7:H:6:ARG:O	7:H:69:ARG:HG2	2.02	0.59
1:A:1245:G:OP1	11:O:13:ASN:ND2	2.35	0.59
1:A:139:G:N2	1:A:141:A:N1	2.44	0.59
1:A:1191:G:P	11:O:18:ARG:HH22	2.26	0.59
28:6:44:ARG:HD3	28:6:47:THR:CG2	2.31	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
26:4:42:PHE:O	26:4:44:THR:N	2.34	0.59
1:A:1171:G:O2'	1:A:1173:G:O4'	2.19	0.59
1:A:1113:U:H2'	1:A:1114:G:C8	2.38	0.59
1:A:2836:U:H2'	1:A:2837:G:C8	2.37	0.59
10:N:34:THR:OG1	10:N:35:VAL:N	2.34	0.59
1:A:1582:C:HO2'	1:A:1586:A:H8	1.48	0.59
1:A:1496:A:H8	1:A:1577:C:HO2'	1.49	0.59
5:F:3:GLU:HB3	5:F:24:LEU:CD2	2.31	0.59
5:F:26:ALA:C	5:F:27:GLU:HG3	2.22	0.59
1:A:1645:G:H5''	1:A:1646:C:H5'	1.83	0.59
15:R:21:GLU:O	15:R:91:ARG:NH2	2.36	0.59
28:6:46:HIS:CD2	28:6:46:HIS:H	2.20	0.59
6:G:113:ARG:HD3	6:G:140:ILE:O	2.03	0.59
1:A:2757:A:C2	7:H:67:LEU:HD11	2.38	0.59
3:D:25:THR:O	3:D:27:THR:N	2.36	0.59
1:A:1175:U:O2'	1:A:1176:G:N3	2.29	0.59
3:D:70:TRP:HZ3	3:D:146:GLU:CD	2.06	0.59
1:A:1024:G:H3'	1:A:1025:G:H5''	1.85	0.59
1:A:654(F):C:O2	1:A:654(P):G:N2	2.35	0.59
7:H:135:GLY:O	7:H:137:ASP:N	2.35	0.59
1:A:2108:C:O2	1:A:2181:G:N2	2.24	0.59
2:B:39:A:C6	26:4:1:MET:HB2	2.37	0.59
17:2:49:THR:CB	17:2:50:PRO:HD3	2.18	0.59
26:4:37:SER:OG	26:4:38:LYS:N	2.33	0.59
1:A:880:G:O6	1:A:897:C:N4	2.36	0.59
26:4:14:ILE:HG13	26:4:33:VAL:HG11	1.84	0.59
1:A:1070:A:C5'	1:A:1071:G:H5''	2.33	0.59
7:H:163:TYR:HE2	7:H:169:VAL:HG11	1.68	0.59
21:V:70:LEU:O	21:V:89:PHE:N	2.23	0.59
14:Q:85:VAL:HG22	14:Q:110:LEU:HB3	1.84	0.59
11:O:46:LYS:HD3	11:O:51:PHE:CD1	2.38	0.59
1:A:2133:G:H2'	1:A:2157:G:N1	2.18	0.59
1:A:2849:U:H4'	1:A:2868:A:C2	2.38	0.59
6:G:38:VAL:HG22	6:G:93:THR:HG23	1.85	0.59
1:A:1593:G:H2'	1:A:1594:G:H8	1.67	0.59
7:H:61:HIS:O	7:H:65:HIS:N	2.28	0.59
1:A:536:A:OP1	16:1:53:ARG:NH1	2.35	0.59
8:K:130:TYR:HB3	8:K:136:VAL:HG13	1.85	0.59
10:N:75:SER:OG	15:R:74:ARG:NH1	2.36	0.59
29:7:32:LYS:NZ	29:7:32:LYS:HB3	2.18	0.59
28:6:44:ARG:O	28:6:45:LYS:HG3	2.03	0.58
4:E:52:LEU:O	4:E:75:VAL:N	2.36	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:43:ARG:NH1	3:D:44:ASN:ND2	2.51	0.58
1:A:1111:A:O2'	7:H:3:ARG:N	2.36	0.58
1:A:1567:A:H5'	3:D:58:HIS:CD2	2.38	0.58
7:H:74:ASN:OD1	7:H:74:ASN:N	2.35	0.58
4:E:68:ALA:O	4:E:69:LYS:C	2.41	0.58
15:R:24:PRO:HA	15:R:49:VAL:HG13	1.85	0.58
1:A:2306:C:H3'	1:A:2307:G:H5''	1.84	0.58
1:A:2562:U:H1'	10:N:23:ARG:HD3	1.84	0.58
18:S:73:ALA:HB3	18:S:106:ILE:HG12	1.85	0.58
4:E:23:VAL:HG21	4:E:183:LEU:CG	2.32	0.58
11:O:47:ASP:CB	11:O:48:PRO:HA	2.30	0.58
1:A:2130:U:H4'	1:A:2134:A:H5'	1.85	0.58
1:A:779:U:OP1	3:D:49:ILE:HG22	2.02	0.58
3:D:146:GLU:OE1	3:D:190:TYR:N	2.18	0.58
1:A:328:U:H4'	20:U:68:HIS:ND1	2.17	0.58
8:K:68:LEU:HA	8:K:71:ILE:HG22	1.85	0.58
2:B:89(A):A:H5'	2:B:90:C:OP2	2.04	0.58
16:1:92:ARG:CZ	17:2:11:GLN:H	2.15	0.58
4:E:37:ARG:HA	4:E:42:ASP:OD2	2.03	0.58
1:A:2889:C:H3'	1:A:2891:G:H8	1.68	0.58
1:A:1171:G:H1	1:A:1174:A:H61	1.51	0.58
1:A:2843:G:H1	1:A:2874:C:H42	1.51	0.58
7:H:2:SER:O	7:H:4:ILE:N	2.37	0.58
1:A:654(O):G:H2'	1:A:654(P):G:C8	2.38	0.58
1:A:2387:U:O2'	22:3:41:ARG:NH1	2.36	0.58
21:V:19:ARG:NE	21:V:84:GLU:OE2	2.36	0.58
1:A:592:G:H21	30:8:4:MET:HE1	1.66	0.58
16:1:92:ARG:NH1	17:2:11:GLN:O	2.37	0.58
11:O:62:LEU:HG	30:8:25:MET:O	1.98	0.58
6:G:167:GLU:O	6:G:170:ARG:HB3	2.04	0.58
1:A:2327:A:H2'	1:A:2328:A:C8	2.39	0.58
1:A:1858:G:O2'	1:A:1884:A:N6	2.36	0.58
9:M:58:ASP:N	9:M:58:ASP:OD1	2.36	0.58
17:2:35:LEU:HG	17:2:37:VAL:CG1	2.33	0.58
1:A:2839:G:C5'	13:0:46:GLY:HA2	2.34	0.58
4:E:174:ASP:OD1	4:E:175:VAL:N	2.36	0.58
4:E:7:VAL:O	4:E:26:ILE:HG23	2.03	0.58
1:A:889:C:N3	1:A:890:A:O2'	2.36	0.58
1:A:1210:A:H5''	1:A:1211:U:H3'	1.86	0.58
1:A:1478:G:H2'	1:A:1479:G:H8	1.69	0.58
21:V:45:ASP:O	21:V:49:ARG:HG2	2.03	0.58
1:A:242:G:O5'	30:8:3:LYS:HE3	2.04	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
17:2:5:VAL:HB	17:2:37:VAL:HG12	1.86	0.58
3:D:69:ARG:C	3:D:71:ASP:H	2.07	0.58
6:G:104:GLU:HG2	26:4:23:GLU:HG2	1.85	0.58
1:A:1059:G:H3'	1:A:1060:U:H2'	1.84	0.58
1:A:1899:G:O2'	1:A:1900:A:H5''	2.04	0.58
1:A:1728:G:C6	1:A:1730:U:H5'	2.38	0.58
4:E:4:ILE:CD1	4:E:28:ALA:HB1	2.34	0.58
1:A:140:A:H8	1:A:1408:C:HO2'	1.51	0.58
1:A:960:A:H61	12:P:83:MET:HE2	1.68	0.58
1:A:221:A:N1	1:A:265:A:O2'	2.33	0.58
1:A:2053:G:H5'	4:E:144:ARG:O	2.04	0.58
1:A:806:C:O2	1:A:2444:G:O2'	2.22	0.57
12:P:65:PHE:O	12:P:67:ARG:N	2.37	0.57
1:A:463:G:N2	1:A:466:A:OP2	2.33	0.57
1:A:270(R):G:H21	23:Z:78:LYS:HD3	1.67	0.57
1:A:2823:A:OP1	4:E:113:PHE:HB2	2.04	0.57
1:A:654(I):C:N4	1:A:654(M):C:O2	2.36	0.57
1:A:2404:C:O3'	11:O:77:ARG:NH2	2.37	0.57
1:A:1093:G:N2	1:A:1098:A:H62	2.02	0.57
1:A:1019:U:HO2'	1:A:1021:A:H2	1.49	0.57
1:A:2816:C:O2	1:A:2883:A:O2'	2.21	0.57
1:A:270(L):U:O2'	1:A:270(M):U:OP1	2.21	0.57
1:A:1753:G:OP2	15:R:115:ARG:NH2	2.37	0.57
1:A:2370:G:H2'	1:A:2371:G:O4'	2.05	0.57
1:A:1050:A:H3'	1:A:1051:G:H8	1.69	0.57
1:A:1071:G:H2'	1:A:1072:C:C6	2.39	0.57
23:Z:86:SER:N	23:Z:87:PRO:HD2	2.20	0.57
15:R:92:GLY:HA2	15:R:116:ALA:HA	1.85	0.57
11:O:62:LEU:HD22	30:8:27:THR:HG22	1.87	0.57
1:A:1037:G:N1	1:A:1118:C:N3	2.32	0.57
14:Q:66:ALA:HA	14:Q:69:VAL:HG12	1.85	0.57
1:A:1030:G:H1	1:A:1124:C:H42	1.52	0.57
6:G:97:ASP:HA	6:G:100:TRP:CD1	2.39	0.57
5:F:2:LYS:O	5:F:24:LEU:CG	2.46	0.57
2:B:66:A:H61	2:B:108:C:H5''	1.70	0.57
1:A:1856:G:H1	1:A:1886:C:H42	1.52	0.57
22:3:25:ARG:HD2	22:3:29:GLN:NE2	2.19	0.57
1:A:1819:A:H4'	1:A:1820:U:O5'	2.04	0.57
9:M:38:HIS:NE2	9:M:50:ASP:OD2	2.24	0.57
1:A:666:G:OP1	11:O:47:ASP:O	2.22	0.57
26:4:21:VAL:HG22	26:4:22:ILE:H	1.69	0.57
8:K:91:SER:HB2	8:K:119:PRO:HB2	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:G:77:ILE:H	6:G:82:LEU:HB2	1.70	0.57
1:A:1472:A:H2'	1:A:1473:G:O4'	2.05	0.57
16:1:61:TRP:CZ3	16:1:94:ASN:HB2	2.40	0.57
11:O:64:LYS:O	11:O:64:LYS:CG	2.52	0.57
6:G:108:ASN:HB3	26:4:38:LYS:HD3	1.87	0.57
1:A:894:C:H5'	1:A:895:U:OP2	2.05	0.57
1:A:1052:C:H42	1:A:1106:G:H1	1.51	0.57
1:A:531:C:OP1	1:A:561:G:N2	2.38	0.57
1:A:1192:G:OP2	11:O:18:ARG:NH2	2.37	0.57
11:O:62:LEU:CD1	30:8:25:MET:CA	2.81	0.57
1:A:1021:A:H62	1:A:1141:U:H3	1.52	0.57
7:H:92:ILE:HG22	7:H:93:GLY:N	2.18	0.57
17:2:85:LYS:HE3	17:2:87:HIS:CD2	2.40	0.57
1:A:1534:G:H2'	1:A:1537:C:N4	2.19	0.57
12:P:21:THR:H	12:P:98:LYS:HB2	1.70	0.57
1:A:2394:C:OP1	11:O:63:PRO:HG2	2.04	0.56
6:G:112:PRO:HA	6:G:117:PHE:HD2	1.70	0.56
1:A:2532:G:O2'	1:A:2657:A:N1	2.37	0.56
18:S:59:VAL:HA	18:S:64:MET:H	1.70	0.56
2:B:15:A:H5'	2:B:16:G:H8	1.69	0.56
1:A:247:G:H4'	1:A:386:G:C5	2.40	0.56
1:A:2401:U:H3'	1:A:2402:C:H5''	1.87	0.56
16:1:92:ARG:HD2	17:2:11:GLN:HB2	1.86	0.56
1:A:2168:G:H1	1:A:2170:A:H8	1.53	0.56
7:H:69:ARG:O	7:H:69:ARG:NH1	2.30	0.56
1:A:2401:U:H2'	1:A:2402:C:C6	2.40	0.56
1:A:1155:A:O3'	16:1:55:ARG:NH1	2.38	0.56
1:A:2015:A:H1'	27:5:2:ALA:HA	1.87	0.56
16:1:92:ARG:O	16:1:94:ASN:N	2.38	0.56
4:E:63:LEU:C	4:E:64:LYS:HG2	2.25	0.56
11:O:48:PRO:O	11:O:51:PHE:N	2.39	0.56
1:A:2163:C:H5''	1:A:2171:A:H8	1.68	0.56
1:A:2747:G:O6	1:A:2755:C:H5''	2.05	0.56
1:A:587:C:OP2	11:O:21:ARG:NH2	2.39	0.56
1:A:300:A:OP1	20:U:84:ARG:NH2	2.19	0.56
1:A:654(D):G:H1	1:A:654(Q):C:N4	2.04	0.56
1:A:274:G:H2'	1:A:275:G:C8	2.39	0.56
14:Q:61:ASN:OD1	14:Q:64:GLU:N	2.35	0.56
1:A:2576:G:O2'	1:A:2579:C:OP2	2.18	0.56
6:G:72:ARG:NE	6:G:85:GLY:O	2.35	0.56
1:A:796:C:H2'	1:A:797:C:C6	2.40	0.56
7:H:42:ARG:NH2	7:H:43:VAL:O	2.38	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:F:5:ALA:O	5:F:7:TYR:N	2.38	0.56
1:A:1085:A:O2'	1:A:1086:A:H8	1.88	0.56
1:A:2277:G:OP2	22:3:12:ASN:ND2	2.39	0.56
1:A:1022:G:H22	1:A:1142(A):A:H2	1.50	0.56
1:A:2318:G:N2	14:Q:3:ARG:HB2	2.20	0.56
1:A:300:A:O2'	1:A:318:C:O2	2.23	0.56
3:D:108:PRO:HD2	3:D:111:LEU:HG	1.86	0.56
23:Z:18:ILE:HG12	23:Z:37:ILE:HG13	1.87	0.56
25:X:19:GLN:HE22	25:X:52:HIS:CE1	2.24	0.56
26:4:41:PRO:O	26:4:42:PHE:HB3	2.05	0.56
1:A:286:C:H2'	1:A:287:C:H6	1.71	0.56
1:A:1533:C:C2	1:A:1534:G:H1'	2.40	0.56
20:U:68:HIS:HB3	20:U:71:LYS:HG3	1.87	0.56
1:A:1871:A:H2'	1:A:1872:A:C8	2.40	0.56
1:A:1070:A:H2'	1:A:1096:A:N3	2.20	0.56
1:A:1093:G:H1'	1:A:1099:G:C2	2.41	0.56
1:A:1046:A:H5''	1:A:1047:G:H5'	1.87	0.56
18:S:29:LEU:O	18:S:33:ARG:HG3	2.05	0.56
12:P:111:GLU:OE1	12:P:133:ARG:NH2	2.39	0.56
1:A:1164:G:H1	1:A:1185:C:H42	1.54	0.56
8:K:14:ASP:N	8:K:17:GLN:OE1	2.39	0.56
17:2:37:VAL:HG21	17:2:57:VAL:H	1.70	0.56
28:6:44:ARG:HG3	28:6:45:LYS:N	2.20	0.56
3:D:43:ARG:HD2	3:D:44:ASN:CG	2.26	0.56
1:A:654(B):C:N4	1:A:654(S):G:O6	2.25	0.56
8:K:72:LEU:O	8:K:74:ASN:N	2.39	0.56
24:W:15:LYS:HA	24:W:67:LYS:HD2	1.86	0.56
1:A:67:U:N3	1:A:74:A:H2	2.03	0.56
4:E:14:ILE:HD11	4:E:173:VAL:HG11	1.86	0.56
4:E:11:MET:HE3	4:E:24:THR:HG23	1.86	0.56
4:E:51:PHE:CE2	4:E:52:LEU:HG	2.40	0.56
4:E:71:GLY:O	4:E:73:GLU:HG2	2.06	0.56
12:P:24:GLY:HA2	12:P:101:ARG:HD2	1.86	0.56
21:V:89:PHE:O	21:V:91:LEU:N	2.39	0.56
1:A:2147:G:H2'	1:A:2148:G:O4'	2.05	0.56
1:A:1131:G:O6	1:A:2040:C:H1'	2.06	0.56
17:2:33:VAL:N	17:2:59:ALA:O	2.35	0.56
8:K:125:GLU:HB2	8:K:141:LYS:HD3	1.88	0.56
3:D:34:VAL:CG2	3:D:35:LYS:HZ2	1.79	0.56
1:A:2173:A:N6	1:A:2174:C:O2'	2.38	0.56
1:A:2777:G:OP2	1:A:2781:A:O2'	2.19	0.56
5:F:53:THR:HG22	5:F:56:GLU:HG3	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:M:128:HIS:NE2	9:M:134:ARG:HD3	2.21	0.56
20:U:68:HIS:H	20:U:71:LYS:HZ3	1.53	0.56
1:A:2046:G:H5'	27:5:19:ARG:HG3	1.88	0.56
1:A:1279:G:H4'	13:0:31:HIS:CD2	2.40	0.56
1:A:771:G:OP1	29:7:10:ARG:NH1	2.39	0.56
15:R:129:ARG:HA	15:R:132:LYS:HB2	1.88	0.56
1:A:1936:A:OP2	1:A:1962:C:N4	2.35	0.56
1:A:872:A:P	12:P:5:ARG:HH22	2.29	0.56
19:T:53:LYS:HB3	19:T:82:GLN:HB3	1.88	0.56
1:A:2355:C:H1'	22:3:39:ARG:HH21	1.71	0.56
9:M:104:LYS:HA	9:M:107:LEU:HD12	1.88	0.56
1:A:480:A:OP2	20:U:46:LYS:HD2	2.05	0.56
1:A:620:G:H4'	1:A:621:A:H5''	1.88	0.55
1:A:654(H):G:H3'	1:A:654(I):C:C5'	2.36	0.55
21:V:106:GLY:HA3	21:V:140:ASP:HB3	1.88	0.55
1:A:1638:C:O2	1:A:2698:U:O2'	2.19	0.55
4:E:63:LEU:HD22	4:E:73:GLU:HG3	1.88	0.55
4:E:71:GLY:C	4:E:73:GLU:N	2.59	0.55
20:U:56:PRO:O	20:U:57:GLN:CB	2.41	0.55
1:A:2801:A:H2'	1:A:2802:G:C4'	2.36	0.55
1:A:2666:C:H42	7:H:152:ARG:HH22	1.54	0.55
21:V:127:LYS:NZ	21:V:162:GLU:OE2	2.39	0.55
3:D:31:LYS:HZ2	3:D:94:LEU:HD11	1.70	0.55
21:V:76:LEU:HD23	21:V:76:LEU:H	1.70	0.55
1:A:93:C:C4'	20:U:54:LYS:NZ	2.69	0.55
3:D:44:ASN:N	3:D:44:ASN:OD1	2.37	0.55
17:2:84:LYS:HZ2	17:2:84:LYS:HB2	1.71	0.55
14:Q:105:ALA:O	14:Q:107:GLU:N	2.39	0.55
21:V:5:LEU:HD21	21:V:39:VAL:HB	1.87	0.55
1:A:2584:U:H2'	1:A:2585:U:C6	2.41	0.55
17:2:53:GLU:O	17:2:55:ALA:N	2.36	0.55
3:D:69:ARG:C	3:D:71:ASP:N	2.60	0.55
5:F:28:ILE:HD12	5:F:119:ARG:NE	2.21	0.55
4:E:21:VAL:HG12	4:E:22:PRO:N	2.22	0.55
21:V:157:LEU:HD12	21:V:161:VAL:HA	1.88	0.55
15:R:3:ARG:CZ	15:R:6:LEU:HD13	2.37	0.55
1:A:654(H):G:H3'	1:A:654(I):C:H5''	1.88	0.55
21:V:113:ALA:O	21:V:115:GLY:N	2.39	0.55
1:A:1403:C:OP1	1:A:1522:G:N2	2.35	0.55
1:A:863:A:H2'	1:A:864:G:C8	2.42	0.55
25:X:18:ASP:N	25:X:18:ASP:OD1	2.32	0.55
1:A:2286:A:H4'	1:A:2287:A:O4'	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:O:47:ASP:N	11:O:48:PRO:HA	2.20	0.55
5:F:63:LYS:HZ3	5:F:67:GLN:HE21	1.55	0.55
2:B:18:G:H1	2:B:65:C:N4	1.91	0.55
5:F:126:VAL:O	5:F:196:LEU:N	2.39	0.55
1:A:1657:C:H2'	1:A:1658:C:H6	1.71	0.55
4:E:11:MET:SD	4:E:24:THR:HG21	2.38	0.55
4:E:9:VAL:HG13	4:E:26:ILE:O	2.06	0.55
28:6:19:ARG:HH21	28:6:52:VAL:CG1	2.18	0.55
2:B:42:C:O2	6:G:93:THR:N	2.39	0.55
1:A:483:A:H4'	20:U:49:VAL:HA	1.88	0.55
1:A:1883:G:HO2'	1:A:1884:A:H8	1.54	0.55
22:3:71:ASP:OD1	22:3:72:ARG:N	2.39	0.55
27:5:46:CYS:SG	27:5:48:GLU:HG2	2.46	0.55
7:H:34:GLU:OE1	7:H:34:GLU:N	2.34	0.55
7:H:60:ARG:O	7:H:63:SER:OG	2.20	0.55
1:A:83:G:N2	1:A:103:A:OP2	2.36	0.55
3:D:25:THR:CG2	3:D:82:ILE:H	2.16	0.55
5:F:185:ASP:OD1	5:F:188:ARG:NH2	2.37	0.55
2:B:24:G:H4'	2:B:25:A:C8	2.42	0.55
1:A:2873:A:H8	13:0:6:SER:N	2.03	0.55
1:A:782:A:N7	3:D:221:VAL:HG21	2.21	0.55
17:2:85:LYS:HE3	17:2:87:HIS:HD2	1.72	0.55
11:O:85:LEU:HB3	11:O:114:ILE:HD11	1.89	0.55
2:B:8:U:O3'	14:Q:25:ARG:NH2	2.37	0.55
5:F:125:LEU:HD23	5:F:125:LEU:H	1.72	0.55
11:O:101:VAL:HG23	11:O:106:LEU:HD23	1.88	0.55
18:S:41:LYS:HD2	27:5:25:LEU:HD11	1.88	0.55
7:H:22:GLY:O	7:H:37:VAL:N	2.40	0.55
3:D:72:LYS:NZ	3:D:99:ASP:OD2	2.35	0.55
4:E:66:HIS:CG	4:E:67:PHE:CA	2.88	0.55
26:4:39:CYS:O	26:4:40:HIS:CG	2.60	0.55
1:A:1427:A:H4'	1:A:1428:C:O5'	2.06	0.55
1:A:1434:A:H61	1:A:1558:A:N6	2.04	0.55
6:G:170:ARG:HH22	6:G:182:LYS:HD3	1.70	0.55
11:O:79:ARG:NE	11:O:109:GLY:O	2.38	0.55
7:H:26:VAL:HG21	7:H:76:VAL:HA	1.88	0.55
1:A:1771:C:HO2'	1:A:1786:A:H8	1.55	0.55
4:E:13:ARG:CB	4:E:21:VAL:O	2.54	0.55
16:1:75:ASN:HB2	16:1:78:THR:HG23	1.89	0.55
1:A:2820:A:O2'	1:A:2821:A:OP1	2.24	0.55
1:A:1186:G:H2'	1:A:1187:G:O4'	2.07	0.55
1:A:1449(A):G:N2	1:A:1462:C:N3	2.44	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:E:25:VAL:HG12	4:E:26:ILE:N	2.22	0.54
1:A:2345:G:OP2	28:6:39:TYR:HA	2.07	0.54
6:G:109:VAL:O	6:G:113:ARG:HG3	2.07	0.54
1:A:1536:A:OP2	1:A:1537:C:N4	2.40	0.54
4:E:131:ALA:HB1	4:E:135:HIS:HE1	1.72	0.54
9:M:93:THR:O	9:M:94:HIS:ND1	2.41	0.54
1:A:2784:C:O2	4:E:37:ARG:NH2	2.40	0.54
6:G:5:VAL:HG11	6:G:100:TRP:HB2	1.88	0.54
6:G:173:LEU:HB3	6:G:178:PHE:CG	2.42	0.54
9:M:34:LEU:O	9:M:49:GLY:HA3	2.07	0.54
1:A:637:A:OP1	11:O:133:SER:OG	2.14	0.54
3:D:145:VAL:HG13	3:D:191:ALA:HB2	1.90	0.54
4:E:67:PHE:O	4:E:67:PHE:CD2	2.60	0.54
2:B:24:G:N2	2:B:27:C:N3	2.40	0.54
1:A:270(I):G:H2'	1:A:270(J):G:H8	1.73	0.54
3:D:16:MET:HG3	3:D:206:LEU:O	2.07	0.54
1:A:1070:A:H5'	1:A:1071:G:H5''	1.89	0.54
2:B:55:U:H2'	2:B:56:G:C8	2.42	0.54
1:A:2798:C:OP1	1:A:2801:A:N6	2.31	0.54
1:A:2801:A:OP1	1:A:2895:U:O2'	2.17	0.54
1:A:752:A:H3'	29:7:1:MET:SD	2.46	0.54
1:A:1856:G:N2	1:A:1886:C:N3	2.50	0.54
2:B:84:C:OP1	25:X:15:TYR:OH	2.20	0.54
1:A:2815:C:H5'	27:5:29:THR:HG21	1.89	0.54
1:A:747:U:O2	1:A:2014:A:H1'	2.07	0.54
11:O:23:PRO:O	11:O:25:SER:N	2.40	0.54
1:A:1071:G:H2'	1:A:1072:C:H6	1.72	0.54
6:G:10:LYS:HG2	6:G:15:VAL:HG23	1.88	0.54
6:G:97:ASP:HA	6:G:100:TRP:HD1	1.71	0.54
11:O:112:LEU:H	11:O:128:HIS:CE1	2.25	0.54
1:A:861:A:N3	2:B:79:C:O2'	2.35	0.54
1:A:2887:U:H2'	1:A:2888:C:H6	1.72	0.54
11:O:47:ASP:H	11:O:48:PRO:HA	1.72	0.54
26:4:39:CYS:HB3	26:4:41:PRO:CG	2.38	0.54
1:A:1091:G:H2'	1:A:1092:C:C6	2.42	0.54
1:A:547:A:H3'	1:A:548:A:H8	1.72	0.54
1:A:1114:G:H2'	1:A:1115:G:C8	2.42	0.54
15:R:65:LYS:HD2	15:R:67:SER:HB2	1.90	0.54
1:A:259:G:H21	1:A:621:A:H8	1.56	0.54
14:Q:65:VAL:HA	14:Q:68:GLN:HG3	1.88	0.54
10:N:8:LEU:HD13	10:N:82:ASN:HB3	1.90	0.54
7:H:140:LYS:O	7:H:144:VAL:HG23	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
21:V:9:TYR:CE1	21:V:35:ARG:HD3	2.42	0.54
22:3:51:VAL:N	22:3:62:LEU:HD12	2.23	0.54
1:A:1912:A:H4'	1:A:1913:A:OP1	2.08	0.54
5:F:122:LYS:O	5:F:124:LEU:N	2.39	0.54
1:A:389:G:H22	11:O:72:PRO:HD3	1.72	0.54
7:H:46:GLU:N	7:H:49:VAL:O	2.41	0.54
3:D:38:LYS:HG2	3:D:38:LYS:O	2.07	0.54
21:V:144:LEU:HD22	21:V:174:VAL:HG21	1.89	0.54
1:A:1853:A:N3	1:A:2233:U:O2'	2.35	0.54
7:H:56:SER:OG	7:H:57:ASP:N	2.40	0.54
1:A:1589:C:H2'	1:A:1590:U:H6	1.73	0.54
26:4:39:CYS:HB3	26:4:41:PRO:HD3	1.90	0.54
1:A:1056:G:H5''	1:A:1057:A:H5'	1.89	0.54
1:A:1139:G:O2'	1:A:1143:A:N6	2.31	0.54
11:O:49:ARG:HD2	30:8:59:LYS:CG	2.31	0.54
1:A:779:U:P	3:D:49:ILE:HG22	2.48	0.54
1:A:2795:G:H1'	1:A:2802:G:N1	2.23	0.54
1:A:2795:G:N2	1:A:2802:G:N7	2.56	0.54
1:A:2808:U:H5''	1:A:2891:G:O6	2.08	0.54
2:B:104:A:H2'	2:B:105:G:O4'	2.08	0.54
21:V:134:PRO:O	21:V:136:PHE:N	2.41	0.54
1:A:302:C:H42	1:A:315:G:H1	1.55	0.54
15:R:27:THR:HG23	15:R:90:GLN:HB3	1.89	0.54
1:A:2735:G:H2'	1:A:2736:G:H8	1.71	0.54
24:W:68:ARG:HA	24:W:72:ALA:HB2	1.89	0.54
20:U:37:VAL:HG23	20:U:67:LEU:HB3	1.90	0.54
4:E:23:VAL:HG21	4:E:183:LEU:CD2	2.38	0.54
28:6:17:LYS:HD2	28:6:17:LYS:H	1.64	0.54
1:A:666:G:H5''	11:O:47:ASP:O	2.08	0.54
7:H:42:ARG:HH21	7:H:44:VAL:HB	1.70	0.54
8:K:54:GLN:HA	8:K:57:ARG:HB3	1.90	0.54
1:A:2869:G:H2'	1:A:2870:C:O4'	2.07	0.54
1:A:2316:C:O2'	6:G:128:ARG:NH2	2.40	0.54
19:T:15:GLU:N	19:T:15:GLU:OE1	2.37	0.54
16:1:61:TRP:CD2	16:1:94:ASN:HA	2.43	0.53
4:E:69:LYS:N	4:E:69:LYS:CD	2.70	0.53
2:B:13:A:N1	2:B:69:G:O2'	2.29	0.53
1:A:1111:A:H4'	7:H:3:ARG:HB2	1.90	0.53
7:H:6:ARG:HB2	7:H:6:ARG:NH1	2.23	0.53
1:A:2646:C:H2'	1:A:2647:U:O4'	2.07	0.53
21:V:54:HIS:CG	21:V:101:PRO:HD3	2.43	0.53
7:H:42:ARG:HE	7:H:44:VAL:HG12	1.73	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:307:G:H21	1:A:330:A:H62	1.55	0.53
1:A:1025:G:C4	1:A:1135:C:H1'	2.44	0.53
19:T:49:VAL:HB	19:T:83:VAL:HG21	1.90	0.53
11:O:22:GLY:O	11:O:25:SER:HB3	2.07	0.53
1:A:2751:G:H5''	1:A:2752:C:OP2	2.08	0.53
1:A:2880:C:O2	13:O:93:GLY:N	2.40	0.53
5:F:1:MET:HB2	5:F:2:LYS:HD3	1.90	0.53
1:A:1072:C:H5	1:A:1097:U:H5'	1.73	0.53
24:W:53:LEU:O	24:W:57:ILE:HG13	2.08	0.53
13:O:29:LEU:HB3	13:O:75:LEU:HD11	1.90	0.53
14:Q:24:LEU:HD12	14:Q:41:ASP:HA	1.89	0.53
1:A:2898:U:H2'	1:A:2899:G:C8	2.43	0.53
2:B:18:G:H2'	2:B:19:G:C8	2.44	0.53
1:A:1044:G:O2'	1:A:1111:A:N1	2.39	0.53
5:F:184:TYR:O	5:F:188:ARG:HB2	2.08	0.53
1:A:1188:U:H4'	17:2:79:VAL:CG1	2.36	0.53
3:D:31:LYS:O	3:D:31:LYS:HG3	2.07	0.53
1:A:819:A:OP2	1:A:1187:G:N2	2.22	0.53
1:A:1999:C:H4'	1:A:2723:C:O2	2.08	0.53
1:A:1055:G:H1	1:A:1104:C:H42	1.54	0.53
1:A:1169:G:N2	1:A:1180:C:N3	2.35	0.53
2:B:28:C:N4	2:B:56:G:H1	2.06	0.53
7:H:109:PHE:CZ	7:H:152:ARG:HB2	2.43	0.53
12:P:24:GLY:HA3	12:P:25:ASP:HB2	1.91	0.53
9:M:15:LEU:HD22	9:M:53:VAL:HB	1.90	0.53
1:A:1771:C:O2'	1:A:1786:A:H8	1.91	0.53
1:A:1688:U:O2	1:A:1700:A:H5'	2.08	0.53
17:2:98:GLU:OE1	17:2:100:ARG:NH1	2.39	0.53
1:A:2688:U:H5	1:A:2720:U:OP2	1.90	0.53
4:E:53:PRO:O	4:E:55:ASN:ND2	2.42	0.53
4:E:81:ILE:O	4:E:81:ILE:HG22	2.09	0.53
1:A:855:G:O2'	22:3:27:GLU:OE2	2.25	0.53
1:A:814:C:O3'	17:2:84:LYS:NZ	2.40	0.53
1:A:1011:G:OP1	16:1:75:ASN:HB3	2.08	0.53
7:H:26:VAL:HG11	7:H:75:ALA:HB1	1.90	0.53
1:A:1165:U:H2'	1:A:1166:C:C6	2.44	0.53
24:W:14:ARG:HG3	24:W:15:LYS:HG2	1.91	0.53
1:A:320:A:H4'	1:A:322:A:C8	2.44	0.53
1:A:712:G:H1	1:A:719:C:H42	1.57	0.53
1:A:469:G:O6	29:7:37:LYS:HE2	2.09	0.53
30:8:28:GLY:O	30:8:36:LYS:NZ	2.42	0.53
28:6:47:THR:CG2	28:6:47:THR:O	2.57	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1066:U:H3	1:A:1069:A:H5''	1.74	0.53
1:A:1729:A:O2'	1:A:1731:G:N2	2.42	0.53
1:A:2142:C:H2'	1:A:2143:C:C6	2.44	0.53
22:3:49:LYS:O	22:3:50:ASN:ND2	2.42	0.53
5:F:167:ALA:HB1	5:F:173:VAL:HG11	1.90	0.53
3:D:65:ILE:HD11	3:D:106:ILE:HG22	1.91	0.53
11:O:65:ARG:HB3	11:O:68:GLN:HE22	1.73	0.53
1:A:2115:G:H2'	1:A:2116:G:N7	2.24	0.53
9:M:25:ARG:NH1	9:M:25:ARG:HG3	2.23	0.53
1:A:2068:U:N3	1:A:2430:A:H2	2.03	0.53
1:A:2439:A:H5'	1:A:2439:A:C8	2.44	0.53
14:Q:83:LYS:HZ2	14:Q:84:GLN:H	1.57	0.53
1:A:1540:G:H2'	1:A:1541:U:O4'	2.09	0.53
1:A:1025:G:OP1	1:A:1025:G:H8	1.91	0.53
28:6:14:THR:OG1	28:6:20:ASN:N	2.30	0.53
4:E:66:HIS:HA	4:E:68:ALA:H	1.73	0.53
21:V:59:LEU:HG	21:V:69:THR:OG1	2.09	0.53
1:A:320:A:H4'	1:A:322:A:N7	2.24	0.53
1:A:2099:U:H3	1:A:2190:G:H1	1.55	0.53
4:E:97:LYS:N	4:E:100:GLU:OE1	2.39	0.53
1:A:646:A:H2'	1:A:647:G:O4'	2.09	0.53
1:A:1094:U:O2'	1:A:1096:A:OP1	2.26	0.53
1:A:2754:U:H5'	1:A:2755:C:OP2	2.08	0.53
21:V:127:LYS:O	21:V:162:GLU:HB2	2.08	0.53
1:A:271(B):G:N7	1:A:421:U:H2'	2.24	0.53
1:A:270(I):G:O6	1:A:270(Q):C:N4	2.42	0.53
14:Q:14:VAL:HG11	14:Q:89:ARG:HH11	1.74	0.53
7:H:46:GLU:OE1	7:H:51:ARG:NH1	2.41	0.53
16:1:82:GLY:HA2	16:1:85:LYS:HG3	1.91	0.53
10:N:111:PHE:HB3	10:N:114:ILE:HG13	1.90	0.53
4:E:11:MET:HG3	4:E:24:THR:HA	1.91	0.52
1:A:2133:G:N2	1:A:2158:A:OP2	2.43	0.52
20:U:52:SER:CB	20:U:56:PRO:HA	2.37	0.52
1:A:1169:G:H1	1:A:1180:C:N4	1.95	0.52
1:A:2420:C:OP2	30:8:34:TRP:CE2	2.62	0.52
1:A:1470:G:N2	1:A:1522:G:OP2	2.39	0.52
23:Z:82:LEU:H	23:Z:82:LEU:HD23	1.74	0.52
1:A:511:U:H3'	1:A:512:G:H5''	1.90	0.52
1:A:379:G:N2	23:Z:42:GLN:OE1	2.28	0.52
12:P:37:LEU:HD21	12:P:130:LYS:HE2	1.91	0.52
7:H:10:PRO:HG2	7:H:50:VAL:HG13	1.91	0.52
5:F:2:LYS:HG2	5:F:25:PRO:HD2	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:890:A:H2'	1:A:892:G:N7	2.23	0.52
2:B:13:A:O2'	2:B:14:U:H3'	2.09	0.52
3:D:85:ASP:OD2	3:D:88:ARG:NH1	2.37	0.52
20:U:42:VAL:O	20:U:65:ALA:N	2.29	0.52
1:A:1537:C:H2'	1:A:1538:G:O4'	2.10	0.52
5:F:149:ASP:OD1	5:F:150:GLY:N	2.42	0.52
13:0:55:ALA:HB2	13:0:79:LEU:HD13	1.91	0.52
6:G:150:ASP:OD1	6:G:153:ARG:NH2	2.40	0.52
11:O:127:ALA:O	11:O:147:LEU:N	2.37	0.52
6:G:165:THR:HG23	6:G:168:GLU:HG3	1.91	0.52
1:A:627:A:N7	11:O:84:ASN:ND2	2.50	0.52
9:M:55:VAL:HB	9:M:126:PRO:HA	1.92	0.52
1:A:77:C:H42	1:A:109:G:H1	1.57	0.52
9:M:17:ASP:OD1	9:M:56:ASN:ND2	2.42	0.52
1:A:139:G:N2	1:A:1596:A:H4'	2.24	0.52
29:7:5:TRP:NE1	29:7:7:PRO:HG3	2.24	0.52
1:A:2425:A:H4'	1:A:2426:A:H5''	1.92	0.52
14:Q:53:SER:O	14:Q:56:LEU:N	2.35	0.52
15:R:11:GLU:OE1	15:R:11:GLU:N	2.33	0.52
10:N:89:ASN:OD1	10:N:89:ASN:N	2.42	0.52
15:R:134:GLU:OE2	15:R:134:GLU:N	2.39	0.52
1:A:2155:G:H3'	1:A:2156:G:H8	1.75	0.52
1:A:1063:G:C6	1:A:1064:C:H1'	2.43	0.52
12:P:43:THR:OG1	12:P:45:GLN:HG2	2.09	0.52
1:A:602:G:O2'	1:A:604:G:O2'	2.13	0.52
17:2:68:LYS:HD2	17:2:69:LYS:N	2.25	0.52
1:A:153:C:P	23:Z:88:LYS:HZ1	2.31	0.52
1:A:242:G:C5'	30:8:62:LEU:HD13	2.39	0.52
16:1:13:LYS:O	16:1:17:ILE:HG12	2.08	0.52
1:A:2591:C:OP1	3:D:239:ARG:HD2	2.10	0.52
1:A:2371:G:H4'	28:6:45:LYS:CD	2.40	0.52
1:A:2169:A:N3	1:A:2169:A:H2'	2.25	0.52
1:A:2420:C:H6	1:A:2420:C:OP2	1.92	0.52
1:A:2745:C:H4'	7:H:142:GLY:O	2.10	0.52
2:B:30:C:N3	2:B:54:G:N2	2.42	0.52
1:A:33:U:O2'	1:A:34:C:O2	2.18	0.52
15:R:91:ARG:HD2	15:R:124:ASP:OD2	2.10	0.52
1:A:1449(A):G:H1	1:A:1462:C:H42	1.57	0.52
16:1:98:LEU:HB3	16:1:102:GLU:HB2	1.91	0.52
1:A:17:G:H4'	16:1:25:TRP:CH2	2.44	0.52
4:E:26:ILE:CG2	4:E:27:LEU:H	2.19	0.52
17:2:38:LEU:HB3	17:2:52:VAL:HG12	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2638:G:HO2'	1:A:2639:A:H8	1.56	0.52
1:A:309:G:N3	1:A:329:G:O2'	2.41	0.52
7:H:149:ARG:HH12	7:H:163:TYR:HA	1.74	0.52
30:8:40:GLU:HA	30:8:43:GLN:HB2	1.91	0.52
1:A:854:G:H2'	1:A:855:G:C8	2.45	0.52
1:A:1278:A:O2'	13:0:34:ILE:HD11	2.09	0.52
1:A:1149:G:H2'	1:A:1150:C:C6	2.44	0.52
25:X:52:HIS:CE1	25:X:53:LEU:HD23	2.45	0.52
1:A:2527:C:H42	1:A:2536:G:H1	1.58	0.52
7:H:146:ALA:O	7:H:150:ALA:N	2.33	0.52
1:A:1996:C:OP1	10:N:31:LYS:HE2	2.10	0.52
1:A:491:G:O6	18:S:49:LYS:HE2	2.09	0.52
16:1:61:TRP:CH2	16:1:94:ASN:HB2	2.45	0.52
3:D:35:LYS:H	3:D:35:LYS:HD2	1.72	0.52
28:6:15:GLU:HG3	28:6:47:THR:OG1	2.10	0.52
5:F:3:GLU:HB3	5:F:24:LEU:HD21	1.90	0.52
1:A:2420:C:P	30:8:34:TRP:CD2	3.03	0.52
6:G:77:ILE:HG22	6:G:80:PHE:H	1.75	0.52
26:4:49:PHE:HD2	26:4:50:VAL:HG22	1.74	0.52
10:N:47:ILE:HG13	10:N:48:PRO:HD2	1.91	0.52
26:4:25:TYR:O	26:4:27:THR:N	2.42	0.52
1:A:84:A:OP2	20:U:8:LYS:NZ	2.26	0.52
6:G:16:ARG:O	6:G:20:ILE:HG22	2.10	0.52
3:D:267:SER:O	3:D:269:PHE:N	2.43	0.52
22:3:47:PRO:HG3	22:3:53:MET:HB2	1.91	0.52
11:O:122:PRO:HA	11:O:142:GLY:H	1.74	0.52
1:A:154:G:O6	1:A:172:C:N4	2.41	0.52
1:A:686:G:N2	1:A:788:A:H61	2.08	0.52
26:4:36:CYS:O	26:4:38:LYS:N	2.43	0.52
26:4:14:ILE:HG13	26:4:33:VAL:CG1	2.40	0.52
3:D:44:ASN:HB3	3:D:49:ILE:HA	1.92	0.52
1:A:1651:G:OP1	13:0:40:LYS:HE3	2.09	0.52
1:A:639:U:H3	1:A:649:G:H1	1.58	0.52
3:D:70:TRP:CZ3	3:D:146:GLU:CD	2.83	0.52
1:A:71:A:H4'	1:A:72:U:H5''	1.91	0.52
1:A:271:G:H2'	1:A:272:G:C8	2.45	0.52
1:A:5:A:H2'	1:A:6:A:H8	1.75	0.52
1:A:2162:G:H2'	1:A:2163:C:C6	2.41	0.52
8:K:75:LEU:HD12	8:K:76:THR:H	1.75	0.52
14:Q:25:ARG:HH11	14:Q:25:ARG:HB2	1.75	0.52
8:K:68:LEU:O	8:K:70:GLU:N	2.43	0.52
1:A:322:A:H5'	1:A:340:A:H1'	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
24:W:13:ALA:HA	24:W:16:LEU:HD21	1.92	0.52
5:F:164:ARG:NH1	5:F:177:ALA:HB2	2.25	0.52
6:G:55:LYS:NZ	6:G:148:MET:SD	2.80	0.52
15:R:119:LYS:O	15:R:123:GLN:HG3	2.10	0.52
26:4:51:ASP:OD1	26:4:51:ASP:N	2.43	0.52
5:F:3:GLU:CB	5:F:24:LEU:HD21	2.40	0.51
11:O:52:GLU:OE1	11:O:53:GLY:N	2.42	0.51
1:A:2006:C:O2'	1:A:2823:A:N3	2.42	0.51
1:A:2262:U:OP2	22:3:19:LYS:NZ	2.41	0.51
6:G:49:ASP:OD2	6:G:51:ARG:NH1	2.42	0.51
1:A:1757:U:O2	1:A:1762:A:N6	2.19	0.51
1:A:1754:C:OP1	15:R:96:ARG:NH1	2.43	0.51
1:A:1899:G:N2	1:A:1902:C:N4	2.54	0.51
1:A:1112:G:H5'	7:H:3:ARG:CZ	2.41	0.51
15:R:6:LEU:HA	15:R:9:LEU:HB2	1.92	0.51
8:K:76:THR:O	8:K:78:THR:OG1	2.28	0.51
28:6:46:HIS:CD2	28:6:46:HIS:N	2.78	0.51
1:A:2512:C:H2'	1:A:2513:G:O4'	2.10	0.51
1:A:616:A:C8	5:F:176:LEU:HD11	2.46	0.51
4:E:8:LYS:HB3	4:E:192:ASN:HA	1.90	0.51
4:E:60:ASN:HA	4:E:63:LEU:HD21	1.92	0.51
1:A:1087:G:H1	1:A:1102:C:N4	2.09	0.51
1:A:1171:G:H1	1:A:1174:A:N6	2.08	0.51
9:M:128:HIS:O	9:M:130:HIS:ND1	2.40	0.51
11:O:30:THR:CG2	11:O:35:HIS:H	2.23	0.51
1:A:601:C:O2'	5:F:104:LYS:NZ	2.44	0.51
28:6:47:THR:O	28:6:48:VAL:C	2.49	0.51
1:A:2115:G:H2'	1:A:2116:G:C5	2.45	0.51
7:H:4:ILE:HG21	7:H:6:ARG:HH21	1.76	0.51
7:H:67:LEU:O	7:H:71:LEU:HB3	2.09	0.51
23:Z:87:PRO:O	23:Z:91:LYS:N	2.42	0.51
6:G:60:LEU:O	6:G:64:THR:HG22	2.10	0.51
1:A:1812:A:H2'	1:A:1813:G:C8	2.46	0.51
10:N:24:VAL:HB	10:N:33:ALA:HB2	1.92	0.51
4:E:66:HIS:NE2	4:E:67:PHE:HB2	2.24	0.51
4:E:72:VAL:CG1	4:E:72:VAL:O	2.58	0.51
4:E:37:ARG:NH1	4:E:80:GLU:OE2	2.37	0.51
1:A:1063:G:C4	1:A:1076:C:C2	2.98	0.51
1:A:1094:U:H5'	1:A:1098:A:H61	1.74	0.51
1:A:1486:A:H2'	1:A:1487:G:H8	1.76	0.51
7:H:23:ARG:HA	7:H:36:PRO:HA	1.93	0.51
15:R:45:PHE:CD2	15:R:74:ARG:HD2	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:G:76:SER:HA	6:G:82:LEU:HB3	1.90	0.51
1:A:6:A:N3	9:M:131:GLN:HG3	2.26	0.51
8:K:1:MET:N	8:K:21:VAL:O	2.39	0.51
12:P:19:GLY:H	12:P:98:LYS:HZ3	1.57	0.51
4:E:201:THR:HG21	4:E:203:LYS:HE2	1.93	0.51
2:B:83:G:H4'	25:X:52:HIS:CG	2.46	0.51
16:1:49:HIS:HA	16:1:52:ARG:HB2	1.92	0.51
1:A:2641:G:O3'	9:M:76:SER:OG	2.27	0.51
4:E:119:ARG:HG2	4:E:160:TYR:HB2	1.92	0.51
1:A:2232:U:P	23:Z:40:ARG:HH12	2.33	0.51
5:F:83:PHE:O	5:F:85:GLY:N	2.44	0.51
6:G:106:LEU:HA	6:G:110:ALA:HB3	1.92	0.51
1:A:1063:G:C2	1:A:1064:C:H4'	2.45	0.51
17:2:65:GLY:O	17:2:91:TYR:N	2.39	0.51
21:V:103:ARG:N	21:V:137:ILE:O	2.36	0.51
6:G:96:ARG:O	6:G:98:ARG:N	2.40	0.51
4:E:109:LYS:O	4:E:111:ARG:NH2	2.44	0.51
4:E:128:SER:OG	4:E:129:HIS:N	2.43	0.51
1:A:769:G:H2'	1:A:770:G:H8	1.75	0.51
12:P:138:ASP:N	12:P:138:ASP:OD1	2.44	0.51
17:2:22:VAL:HG22	17:2:23:GLU:H	1.76	0.51
1:A:546:C:H2'	1:A:547:A:O4'	2.10	0.51
1:A:2542:A:H1'	1:A:2543:G:C8	2.46	0.51
1:A:1567:A:O2'	3:D:63:ARG:NH2	2.44	0.51
15:R:24:PRO:HD3	15:R:52:ILE:HG13	1.93	0.51
14:Q:15:ARG:NH1	14:Q:90:GLY:HA2	2.26	0.51
12:P:6:ARG:O	12:P:7:MET:HG2	2.10	0.51
1:A:1991:U:H2'	1:A:1992:G:H5''	1.93	0.51
4:E:11:MET:HE3	4:E:187:ALA:H	1.76	0.51
11:O:62:LEU:CD2	30:8:27:THR:HG23	2.38	0.51
5:F:3:GLU:O	5:F:5:ALA:N	2.44	0.51
1:A:2801:A:H2'	1:A:2802:G:O4'	2.11	0.51
1:A:1478:G:H2'	1:A:1479:G:C8	2.45	0.51
1:A:1856:G:H1	1:A:1886:C:N4	2.09	0.51
1:A:1846:G:H1	1:A:1894:C:H42	1.59	0.51
12:P:34:LEU:HD11	12:P:129:THR:HB	1.93	0.51
1:A:1864:U:OP1	1:A:2410:G:O2'	2.23	0.51
1:A:2031:A:C6	1:A:2498:C:H1'	2.46	0.51
12:P:11:LYS:NZ	12:P:87:LYS:O	2.43	0.51
30:8:61:LEU:HD13	30:8:62:LEU:HD12	1.92	0.51
13:0:104:ARG:HD2	13:0:109:ALA:HB3	1.93	0.51
7:H:96:ALA:HB1	7:H:99:VAL:HG21	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:670:A:H5''	11:O:42:SER:O	2.11	0.51
1:A:2730:C:O2'	4:E:168:MET:O	2.28	0.51
28:6:14:THR:CB	28:6:20:ASN:H	2.22	0.50
26:4:16:CYS:SG	26:4:18:CYS:N	2.80	0.50
1:A:1054:A:H2	1:A:1084:A:N1	2.09	0.50
1:A:2748:A:H2'	1:A:2749:A:C8	2.45	0.50
6:G:27:ASN:OD1	6:G:28:VAL:N	2.44	0.50
14:Q:83:LYS:O	14:Q:110:LEU:N	2.41	0.50
1:A:635:C:H2'	1:A:636:G:O4'	2.12	0.50
20:U:37:VAL:O	20:U:67:LEU:N	2.42	0.50
1:A:207:A:H2'	1:A:208:C:O4'	2.11	0.50
17:2:35:LEU:O	17:2:37:VAL:HG22	2.11	0.50
3:D:35:LYS:HE3	3:D:64:ILE:CB	2.41	0.50
28:6:27:LYS:HZ3	28:6:28:ARG:NH1	2.08	0.50
28:6:39:TYR:O	28:6:41:PRO:HD3	2.12	0.50
1:A:2637:U:H5''	4:E:82:ARG:HH21	1.75	0.50
17:2:84:LYS:HG3	17:2:85:LYS:HB2	1.92	0.50
6:G:69:ALA:HB3	6:G:91:ARG:HH21	1.76	0.50
1:A:1266:G:O4'	18:S:15:ARG:NH2	2.43	0.50
1:A:863:A:H2'	1:A:864:G:H8	1.75	0.50
3:D:4:LYS:HB3	3:D:18:VAL:HG12	1.93	0.50
4:E:23:VAL:O	4:E:25:VAL:N	2.44	0.50
28:6:27:LYS:HZ3	28:6:28:ARG:HH12	1.60	0.50
11:O:49:ARG:CZ	30:8:59:LYS:HG2	2.41	0.50
5:F:64:ILE:O	5:F:65:TRP:HD1	1.94	0.50
1:A:1061:U:H4'	1:A:1070:A:O2'	2.10	0.50
1:A:2657:A:O3'	7:H:160:LYS:NZ	2.44	0.50
1:A:2803:C:H2'	1:A:2804:C:O4'	2.11	0.50
2:B:38:C:O2	2:B:48:A:H1'	2.11	0.50
3:D:85:ASP:OD1	3:D:87:ASN:ND2	2.44	0.50
24:W:38:GLN:HB3	24:W:44:LEU:O	2.12	0.50
4:E:96:PHE:O	4:E:175:VAL:HG11	2.10	0.50
8:K:1:MET:N	8:K:20:ASP:OD1	2.28	0.50
1:A:494:G:OP1	18:S:8:ARG:NH1	2.37	0.50
16:1:92:ARG:HG2	16:1:95:LEU:HB2	1.93	0.50
1:A:2138:C:C2	1:A:2154:G:C2	2.99	0.50
1:A:2893:G:H4'	1:A:2894:G:O5'	2.11	0.50
1:A:2748:A:N7	1:A:2753:A:N6	2.60	0.50
1:A:1542:G:H3'	1:A:1543:A:C5'	2.40	0.50
21:V:41:LEU:O	21:V:45:ASP:N	2.27	0.50
8:K:27:ARG:HD2	23:Z:71:TYR:CE1	2.47	0.50
21:V:116:VAL:N	21:V:179:ASP:OD1	2.44	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:254:G:N7	30:8:5:LYS:HE2	2.26	0.50
15:R:77:PRO:HB2	15:R:80:SER:HB2	1.93	0.50
11:O:71:VAL:HG13	11:O:72:PRO:N	2.25	0.50
28:6:15:GLU:OE2	28:6:16:CYS:O	2.30	0.50
1:A:1069:A:H3'	1:A:1073:A:H62	1.77	0.50
1:A:1087:G:O6	1:A:1089:G:N2	2.43	0.50
21:V:127:LYS:N	21:V:162:GLU:O	2.44	0.50
2:B:118:G:H3'	2:B:119:A:C8	2.45	0.50
23:Z:91:LYS:O	23:Z:93:GLU:N	2.45	0.50
7:H:137:ASP:OD2	7:H:139:GLN:N	2.44	0.50
1:A:974:G:O2'	1:A:975:G:N7	2.34	0.50
1:A:582:G:H2'	1:A:583:G:C8	2.47	0.50
6:G:75:LYS:HA	6:G:84:LYS:HE2	1.94	0.50
7:H:41:MET:SD	7:H:41:MET:N	2.84	0.50
1:A:389:G:N2	11:O:71:VAL:HG12	2.26	0.50
4:E:67:PHE:O	4:E:68:ALA:C	2.49	0.50
2:B:66:A:H61	2:B:107:U:H2'	1.76	0.50
4:E:13:ARG:HB2	4:E:21:VAL:O	2.12	0.50
7:H:8:PRO:O	7:H:69:ARG:NE	2.41	0.50
1:A:2875:C:H4'	15:R:5:ALA:CB	2.41	0.50
1:A:2120:G:H1	1:A:2178:C:N4	2.08	0.50
3:D:10:THR:OG1	3:D:13:ARG:HB2	2.11	0.50
13:O:53:HIS:ND1	13:O:94:TYR:OH	2.32	0.50
5:F:63:LYS:HZ3	5:F:67:GLN:NE2	2.08	0.50
1:A:1331:A:O2'	1:A:1332:G:H8	1.94	0.50
1:A:1175:U:O2	1:A:1176:G:N1	2.44	0.50
23:Z:92:LYS:NZ	23:Z:97:LEU:HD21	2.27	0.50
1:A:2472:G:N2	1:A:2477:C:OP1	2.44	0.50
21:V:91:LEU:HD22	21:V:130:PRO:HG3	1.94	0.50
6:G:145:THR:OG1	6:G:147:ASP:OD1	2.29	0.50
1:A:2378:A:H4'	14:Q:23:ARG:NH1	2.27	0.50
14:Q:78:LEU:HD11	14:Q:107:GLU:HB3	1.94	0.50
1:A:270(L):U:H3'	1:A:270(M):U:H5''	1.92	0.50
1:A:2086:U:H2'	1:A:2087:G:C8	2.47	0.50
1:A:1295:C:O4'	13:O:23:ASN:ND2	2.38	0.50
4:E:81:ILE:O	4:E:82:ARG:O	2.30	0.50
1:A:1110:G:H2'	1:A:1111:A:H8	1.76	0.50
21:V:29:TYR:CE1	21:V:87:ASP:HB3	2.46	0.50
1:A:1155:A:O2'	1:A:1156:A:H2'	2.11	0.50
1:A:1638:C:H4'	1:A:2710:C:O2	2.11	0.50
1:A:2264:C:N4	22:3:15:ASP:OD2	2.45	0.50
17:2:48:GLY:O	17:2:49:THR:O	2.30	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:E:76:ARG:HG3	4:E:195:LEU:HD22	1.94	0.50
1:A:2115:G:H4'	1:A:2166:G:C8	2.47	0.50
1:A:1071:G:C8	1:A:1097:U:H4'	2.47	0.50
1:A:2746:U:H4'	7:H:138:LYS:HG3	1.93	0.50
1:A:2799:A:H5''	1:A:2801:A:OP2	2.12	0.50
1:A:2293:C:O3'	14:Q:89:ARG:NH2	2.28	0.50
4:E:120:TRP:CG	4:E:155:LYS:HB3	2.46	0.50
1:A:2505:G:O6	1:A:2576:G:H2'	2.12	0.50
1:A:2845:G:O2'	1:A:2846:G:H5'	2.11	0.50
6:G:56:ALA:HA	6:G:59:GLU:HG2	1.93	0.50
4:E:147:PRO:HB2	4:E:149:ARG:HG2	1.94	0.50
4:E:24:THR:O	4:E:25:VAL:O	2.30	0.49
1:A:2124:G:C6	1:A:2125:G:H1'	2.47	0.49
1:A:1088:A:O3'	1:A:1089:G:H8	1.95	0.49
1:A:1657:C:H4'	4:E:133:LYS:HB3	1.92	0.49
14:Q:41:ASP:OD2	14:Q:44:LYS:NZ	2.44	0.49
12:P:12:GLN:HG2	12:P:73:PRO:HD2	1.92	0.49
1:A:375:C:H42	1:A:399:G:H1	1.59	0.49
1:A:920:G:H2'	1:A:921:G:H8	1.77	0.49
1:A:2689:U:H4'	1:A:2690:C:O5'	2.11	0.49
17:2:47:VAL:O	17:2:48:GLY:O	2.30	0.49
1:A:882:G:H1	1:A:894:C:H42	1.59	0.49
1:A:548:A:C2	1:A:549:G:H1'	2.47	0.49
12:P:52:VAL:O	12:P:56:ARG:HB2	2.12	0.49
2:B:37:C:N3	2:B:48:A:O2'	2.45	0.49
6:G:119:GLY:HA3	6:G:180:PHE:O	2.12	0.49
2:B:70:C:H2'	2:B:71:C:H6	1.77	0.49
1:A:2427:C:H5''	1:A:2428:G:OP1	2.13	0.49
25:X:13:ILE:HD12	25:X:13:ILE:H	1.78	0.49
1:A:389:G:H22	11:O:72:PRO:CD	2.24	0.49
11:O:62:LEU:HD11	30:8:25:MET:CB	2.40	0.49
4:E:67:PHE:CE2	4:E:69:LYS:HD3	2.48	0.49
1:A:2445:G:OP1	5:F:74:ARG:NH2	2.46	0.49
26:4:18:CYS:N	26:4:19:GLY:HA2	2.27	0.49
5:F:65:TRP:HB3	5:F:66:PRO:HD2	1.94	0.49
1:A:1106:G:C2	1:A:1107:G:C4	3.01	0.49
1:A:629:G:H4'	1:A:650:C:O2	2.13	0.49
1:A:1448:G:H1'	1:A:1528:A:H62	1.77	0.49
1:A:1204:A:O2'	1:A:1205:U:OP2	2.30	0.49
1:A:654(E):C:N4	1:A:654(P):G:H1	2.10	0.49
1:A:1223:C:OP2	17:2:88:ARG:NH2	2.45	0.49
12:P:116:GLU:OE2	12:P:119:ARG:NE	2.44	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1405:U:H2'	1:A:1406:U:C6	2.48	0.49
3:D:26:LYS:HD2	3:D:26:LYS:H	1.77	0.49
1:A:1069:A:H4'	1:A:1096:A:O2'	2.12	0.49
1:A:1097:U:H3'	1:A:1098:A:C8	2.47	0.49
23:Z:89:GLU:O	23:Z:93:GLU:HB2	2.12	0.49
1:A:2335:A:C8	1:A:2337:G:C5	3.01	0.49
1:A:128:C:O5'	29:7:48:LYS:NZ	2.46	0.49
17:2:83:ARG:N	17:2:83:ARG:HD2	2.28	0.49
1:A:2115:G:N2	1:A:2172:U:O4	2.46	0.49
26:4:20:ASN:ND2	26:4:21:VAL:H	2.10	0.49
1:A:1021:A:OP2	9:M:65:LYS:NZ	2.45	0.49
18:S:11:ARG:CZ	18:S:98:LYS:HB3	2.42	0.49
14:Q:66:ALA:O	14:Q:70:GLY:N	2.33	0.49
1:A:224:G:N7	1:A:420:C:H4'	2.28	0.49
3:D:28:GLU:HB3	3:D:29:PRO:HD3	1.94	0.49
6:G:166:ASP:OD1	6:G:166:ASP:N	2.45	0.49
1:A:20:C:OP1	16:1:22:LYS:NZ	2.28	0.49
28:6:16:CYS:O	28:6:17:LYS:O	2.30	0.49
1:A:1051:G:N2	1:A:1052:C:O4'	2.45	0.49
1:A:1057:A:N6	1:A:1058:U:H3	2.10	0.49
5:F:40:GLN:HE22	5:F:182:ASN:HB2	1.76	0.49
1:A:851:U:O2'	25:X:42:ALA:O	2.24	0.49
1:A:2334:G:O6	22:3:74:ARG:NH2	2.46	0.49
1:A:2401:U:H2'	1:A:2402:C:H6	1.75	0.49
1:A:918:A:O2'	2:B:96:G:N2	2.42	0.49
6:G:22:ARG:HH12	6:G:175:LEU:HD21	1.78	0.49
1:A:270(V):G:H2'	1:A:270(W):G:C8	2.47	0.49
28:6:14:THR:CA	28:6:20:ASN:O	2.61	0.49
1:A:1062:G:H22	1:A:1076:C:H42	1.59	0.49
1:A:1072:C:O2	1:A:1092:C:H5	1.95	0.49
1:A:2808:U:H3'	1:A:2891:G:H1	1.78	0.49
1:A:351:G:O3'	1:A:352:G:H8	1.94	0.49
1:A:2212:A:O2'	1:A:2213:U:O5'	2.31	0.49
14:Q:7:TYR:CE2	14:Q:91:PRO:HG2	2.48	0.49
3:D:34:VAL:CB	3:D:35:LYS:HD3	2.43	0.49
4:E:60:ASN:HB3	4:E:63:LEU:CD1	2.25	0.49
5:F:5:ALA:N	5:F:18:ARG:O	2.45	0.49
22:3:12:ASN:HA	22:3:14:ARG:HH21	1.77	0.49
2:B:86:G:N2	2:B:90:C:O2	2.26	0.49
1:A:2542:A:O2'	1:A:2543:G:P	2.71	0.49
1:A:300:A:P	20:U:84:ARG:HH22	2.34	0.49
1:A:2097:C:H2'	1:A:2098:U:O4'	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2145:C:H3'	1:A:2147:G:N2	2.28	0.49
1:A:592:G:H21	30:8:4:MET:CE	2.25	0.49
1:A:2246:G:H2'	1:A:2247:A:C8	2.48	0.49
1:A:26:G:OP1	18:S:80:PRO:HB3	2.11	0.49
1:A:2107:C:H42	1:A:2182:G:H1	1.60	0.49
8:K:128:LEU:O	8:K:138:ILE:N	2.33	0.49
7:H:108:GLY:O	7:H:152:ARG:NH1	2.46	0.49
4:E:179:GLU:HB2	4:E:181:LEU:HD23	1.94	0.49
4:E:116:VAL:O	4:E:118:LYS:N	2.39	0.49
12:P:66:ILE:HG13	12:P:67:ARG:H	1.78	0.49
16:1:98:LEU:HA	16:1:100:VAL:O	2.13	0.49
1:A:363(B):G:H2'	1:A:363(C):G:H8	1.77	0.49
7:H:124:GLU:O	7:H:125:VAL:C	2.51	0.49
4:E:53:PRO:O	4:E:55:ASN:N	2.46	0.49
11:O:48:PRO:O	11:O:49:ARG:C	2.48	0.49
1:A:2061:G:OP1	5:F:68:LYS:CE	2.53	0.49
17:2:91:TYR:O	17:2:91:TYR:CD2	2.62	0.49
1:A:1019:U:H3	1:A:1142(A):A:N6	2.04	0.49
8:K:69:LYS:HA	8:K:136:VAL:HG21	1.94	0.49
12:P:74:TYR:O	12:P:90:VAL:HA	2.12	0.49
6:G:50:ALA:HA	6:G:53:LEU:HB3	1.94	0.49
1:A:2161:C:H2'	1:A:2162:G:H8	1.78	0.48
6:G:105:LYS:CE	26:4:26:SER:HB3	2.42	0.48
1:A:2297:C:N4	1:A:2321:G:O6	2.42	0.48
1:A:988:A:H3'	25:X:11:SER:OG	2.12	0.48
1:A:270(I):G:H2'	1:A:270(J):G:C8	2.48	0.48
6:G:170:ARG:NH2	6:G:182:LYS:HD3	2.27	0.48
21:V:111:VAL:O	21:V:113:ALA:N	2.46	0.48
1:A:702:G:H1	1:A:730:C:H42	1.61	0.48
1:A:2695:C:H2'	1:A:2696:U:C6	2.48	0.48
11:O:37:GLY:HA2	11:O:41:ARG:NH2	2.28	0.48
3:D:35:LYS:CE	3:D:64:ILE:CG1	2.79	0.48
28:6:14:THR:HA	28:6:20:ASN:O	2.13	0.48
11:O:49:ARG:O	11:O:50:ARG:HB2	2.13	0.48
5:F:16:GLY:O	5:F:18:ARG:N	2.46	0.48
26:4:39:CYS:CB	26:4:41:PRO:HD2	2.43	0.48
1:A:892:G:C8	1:A:893:C:C4	3.01	0.48
1:A:1056:G:H5''	1:A:1057:A:C5'	2.43	0.48
21:V:30:ASN:HB2	21:V:33:LEU:HB3	1.94	0.48
1:A:270(I):G:H1	1:A:270(Q):C:H42	1.60	0.48
24:W:33:MET:HG2	24:W:37:PHE:HE1	1.78	0.48
15:R:21:GLU:N	15:R:21:GLU:OE2	2.45	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:E:112:GLY:O	4:E:159:HIS:HA	2.13	0.48
1:A:2899:G:H2'	1:A:2900:A:C8	2.48	0.48
12:P:51:ARG:O	12:P:54:MET:N	2.45	0.48
12:P:20:ALA:HB2	21:V:79:ARG:NH2	2.28	0.48
1:A:392:C:H5''	1:A:409:C:H5''	1.95	0.48
1:A:2155:G:H3'	1:A:2156:G:C8	2.49	0.48
5:F:28:ILE:CD1	5:F:119:ARG:NE	2.69	0.48
5:F:64:ILE:C	5:F:65:TRP:CD1	2.87	0.48
1:A:1086:A:OP1	1:A:1104:C:H1'	2.13	0.48
21:V:59:LEU:HD12	21:V:69:THR:HG21	1.94	0.48
1:A:2271:G:OP1	22:3:18:ALA:HB1	2.13	0.48
14:Q:16:ASN:HA	14:Q:19:LYS:HD2	1.95	0.48
1:A:1567:A:OP2	3:D:84:TYR:OH	2.21	0.48
23:Z:51:VAL:HG23	23:Z:58:ILE:HB	1.95	0.48
4:E:55:ASN:C	4:E:57:LYS:H	2.16	0.48
1:A:2165:G:P	1:A:2166:G:H21	2.35	0.48
5:F:63:LYS:CE	5:F:67:GLN:HB2	2.42	0.48
1:A:1060:U:O4'	1:A:1062:G:H5'	2.14	0.48
1:A:1085:A:C4	1:A:1086:A:C8	3.00	0.48
1:A:2749:A:H1'	7:H:63:SER:HB3	1.95	0.48
1:A:1428:C:O2'	1:A:1569:A:OP2	2.19	0.48
1:A:2150:U:H2'	1:A:2151:G:C8	2.48	0.48
11:O:108:LYS:O	11:O:110:TYR:N	2.43	0.48
7:H:124:GLU:OE1	7:H:124:GLU:N	2.47	0.48
1:A:142:G:H2'	1:A:143:C:H6	1.78	0.48
1:A:631:A:OP1	11:O:64:LYS:NZ	2.46	0.48
28:6:43:CYS:O	28:6:44:ARG:O	2.32	0.48
1:A:2135:A:OP2	1:A:2136:C:N4	2.46	0.48
1:A:2790:A:H4'	1:A:2893:G:H21	1.78	0.48
1:A:2748:A:O5'	7:H:70:THR:HG21	2.13	0.48
1:A:67:U:H3	1:A:74:A:H2	1.56	0.48
1:A:1788:C:H5''	3:D:225:ALA:HB1	1.95	0.48
21:V:117:LEU:HD22	21:V:118:GLN:H	1.78	0.48
25:X:39:ASP:O	25:X:44:ARG:NH2	2.46	0.48
1:A:2113:U:O4	1:A:2168:G:O2'	2.24	0.48
6:G:111:LEU:HB3	6:G:117:PHE:CE2	2.49	0.48
1:A:2674:G:OP1	10:N:26:LYS:NZ	2.45	0.48
23:Z:92:LYS:C	23:Z:94:LEU:H	2.17	0.48
1:A:141:A:C8	1:A:1408:C:H1'	2.48	0.48
1:A:245:G:O3'	11:O:70:GLN:O	2.32	0.48
1:A:246:C:P	11:O:70:GLN:O	2.72	0.48
1:A:343:C:H2'	1:A:344:G:H8	1.77	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1181:C:H2'	1:A:1182:A:C8	2.48	0.48
1:A:956:G:H2'	1:A:957:A:H2'	1.96	0.48
17:2:20:LEU:O	17:2:94:LEU:N	2.29	0.48
1:A:2393:A:H4'	11:O:61:ARG:HA	1.96	0.48
1:A:2114:A:N6	1:A:2115:G:O6	2.47	0.48
1:A:1060:U:H5''	1:A:1061:U:C4	2.49	0.48
3:D:63:ARG:H	3:D:87:ASN:ND2	2.10	0.48
14:Q:10:ARG:O	14:Q:14:VAL:HG13	2.14	0.48
7:H:44:VAL:O	7:H:51:ARG:N	2.40	0.48
1:A:1812:A:H2'	1:A:1813:G:H8	1.78	0.48
6:G:126:ASP:OD2	6:G:130:ASN:ND2	2.46	0.48
18:S:26:GLY:H	18:S:71:VAL:HB	1.79	0.48
1:A:1779:U:OP2	1:A:1784:A:N6	2.36	0.48
4:E:23:VAL:O	4:E:24:THR:OG1	2.30	0.48
20:U:54:LYS:C	20:U:55:TYR:HD2	2.17	0.48
1:A:1071:G:H1'	1:A:1089:G:C2'	2.43	0.48
1:A:330:A:O2'	1:A:331:A:H8	1.97	0.48
1:A:1111:A:O3'	1:A:1112:G:H4'	2.14	0.48
14:Q:14:VAL:O	14:Q:18:ILE:HG23	2.14	0.48
23:Z:91:LYS:HA	23:Z:91:LYS:HZ3	1.79	0.48
24:W:15:LYS:HD2	24:W:67:LYS:NZ	2.29	0.48
1:A:1913:A:H4'	1:A:1914:C:OP1	2.14	0.48
1:A:2080:G:O2'	1:A:2081:C:H5'	2.14	0.48
1:A:2468:G:P	12:P:119:ARG:HH22	2.36	0.48
1:A:1782:C:H1'	1:A:2609:U:H5''	1.95	0.48
5:F:70:THR:HG23	5:F:71:GLY:N	2.28	0.48
21:V:15:PRO:HA	21:V:18:LEU:HD23	1.95	0.48
1:A:856:C:HO2'	1:A:857:C:P	2.34	0.48
1:A:2889:C:H2'	1:A:2891:G:O4'	2.13	0.48
1:A:2467:C:O2	12:P:124:LYS:NZ	2.40	0.48
27:5:3:LYS:HE3	27:5:4:HIS:HB2	1.95	0.48
1:A:2212:A:H4'	1:A:2213:U:C4	2.49	0.48
2:B:33:G:C6	2:B:34:U:C4	3.02	0.48
9:M:30:ILE:O	9:M:34:LEU:HD22	2.14	0.48
1:A:1412:A:H2'	1:A:1413:G:C8	2.49	0.48
30:8:48:PHE:CG	30:8:49:VAL:N	2.82	0.48
8:K:9:LEU:HD11	8:K:12:LEU:HD22	1.96	0.48
1:A:2134:A:C2	1:A:2135:A:C8	3.02	0.48
3:D:27:THR:HB	3:D:83:GLU:HG2	1.96	0.48
27:5:3:LYS:HG2	27:5:4:HIS:N	2.28	0.48
1:A:620:G:N3	1:A:620:G:H5'	2.29	0.48
1:A:1024:G:C3'	1:A:1025:G:H5''	2.44	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
15:R:18:ASP:OD1	15:R:18:ASP:N	2.46	0.48
6:G:115:ARG:O	6:G:117:PHE:N	2.46	0.47
1:A:2790:A:H8	1:A:2790:A:OP2	1.97	0.47
9:M:25:ARG:HH11	9:M:25:ARG:HG3	1.79	0.47
1:A:1140:C:O3'	9:M:25:ARG:NH2	2.47	0.47
2:B:89:G:N3	2:B:89(A):A:H2	2.11	0.47
2:B:55:U:C1'	6:G:29:TRP:HE1	2.27	0.47
10:N:88:ASN:O	10:N:91:LEU:N	2.47	0.47
15:R:107:ASP:O	15:R:111:ARG:NH1	2.47	0.47
1:A:1785:A:H4'	1:A:1982:C:O2'	2.14	0.47
1:A:1505:C:H2'	1:A:1506:C:H6	1.79	0.47
1:A:820:A:N3	1:A:943:U:H4'	2.29	0.47
4:E:72:VAL:O	4:E:73:GLU:C	2.52	0.47
1:A:2155:G:C6	1:A:2156:G:C6	3.01	0.47
4:E:47:VAL:O	4:E:80:GLU:HA	2.14	0.47
17:2:85:LYS:HG3	17:2:87:HIS:HB2	1.96	0.47
16:1:62:ILE:HG13	16:1:76:TYR:CZ	2.49	0.47
27:5:56:LYS:HZ3	27:5:58:LEU:HD11	1.79	0.47
1:A:363(B):G:H2'	1:A:363(C):G:C8	2.49	0.47
1:A:2730:C:O3'	4:E:169:ASN:HB3	2.14	0.47
1:A:2832:U:H3'	1:A:2833:G:C8	2.49	0.47
28:6:14:THR:O	28:6:49:HIS:HB3	2.13	0.47
4:E:36:ARG:HH21	4:E:88:GLY:HA2	1.80	0.47
1:A:219:G:N2	1:A:430:G:O6	2.48	0.47
5:F:185:ASP:HA	5:F:188:ARG:HE	1.78	0.47
1:A:1416:G:O2'	1:A:1417:C:O4'	2.31	0.47
1:A:984:A:H5''	1:A:985:C:H5	1.80	0.47
1:A:948:G:H21	1:A:985:C:P	2.37	0.47
1:A:108:U:H2'	1:A:109:G:H8	1.78	0.47
1:A:686:G:OP1	29:7:11:LYS:HE2	2.14	0.47
1:A:565:C:H4'	1:A:1253:A:C6	2.49	0.47
14:Q:67:ARG:HA	14:Q:104:GLY:HA3	1.96	0.47
3:D:34:VAL:C	3:D:35:LYS:CD	2.56	0.47
11:O:60:MET:O	11:O:61:ARG:HG2	2.09	0.47
4:E:65:GLY:O	4:E:66:HIS:HB2	2.12	0.47
4:E:49:LEU:O	4:E:78:LEU:HB3	2.14	0.47
5:F:24:LEU:CD2	5:F:24:LEU:N	2.75	0.47
1:A:93:C:H5'	1:A:94:G:OP2	2.14	0.47
1:A:1063:G:N1	1:A:1075:C:N3	2.54	0.47
1:A:1111:A:C1'	7:H:2:SER:HA	2.42	0.47
2:B:28:C:H2'	2:B:29:A:O4'	2.14	0.47
18:S:59:VAL:HG23	18:S:65:LEU:N	2.26	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:E:14:ILE:O	4:E:20:ALA:HA	2.15	0.47
1:A:856:C:H3'	1:A:856:C:H6	1.78	0.47
8:K:102:SER:O	8:K:106:GLY:N	2.47	0.47
1:A:459:U:H5''	29:7:40:TRP:CD2	2.49	0.47
1:A:2311:A:C2	6:G:47:LYS:HE3	2.50	0.47
12:P:30:GLY:HA2	12:P:107:ALA:HB2	1.96	0.47
11:O:71:VAL:H	11:O:72:PRO:CD	2.28	0.47
1:A:2393:A:HO2'	30:8:13:ARG:HH12	1.58	0.47
1:A:250:G:C5'	11:O:60:MET:HE1	2.44	0.47
1:A:2135:A:N6	1:A:2156:G:H21	2.12	0.47
1:A:1069:A:O2'	1:A:1072:C:OP2	2.28	0.47
1:A:286:C:H2'	1:A:287:C:C6	2.49	0.47
1:A:2795:G:HO2'	1:A:2802:G:N2	2.12	0.47
2:B:40:U:H1'	2:B:46:A:N1	2.29	0.47
1:A:2145:C:H3'	1:A:2147:G:H21	1.78	0.47
1:A:2187:G:H2'	1:A:2188:C:O4'	2.14	0.47
1:A:1321:A:H2'	1:A:1322:A:O4'	2.14	0.47
1:A:1607:C:H4'	1:A:1608:A:O5'	2.14	0.47
4:E:23:VAL:C	4:E:25:VAL:N	2.66	0.47
16:1:92:ARG:NH2	17:2:11:GLN:H	2.12	0.47
28:6:14:THR:HG21	28:6:19:ARG:CG	2.44	0.47
6:G:101:ILE:C	6:G:105:LYS:HZ3	2.18	0.47
1:A:1069:A:H3'	1:A:1073:A:N6	2.30	0.47
7:H:86:GLU:HA	7:H:132:ARG:HA	1.96	0.47
1:A:2794:C:H2'	1:A:2795:G:O4'	2.15	0.47
3:D:17:THR:OG1	3:D:205:VAL:N	2.45	0.47
1:A:2299:G:C2	1:A:2318:G:H8	2.32	0.47
14:Q:35:ILE:HD11	14:Q:97:ARG:NE	2.27	0.47
8:K:78:THR:HG21	8:K:104:GLN:HG3	1.96	0.47
1:A:1786:A:C2	1:A:2606:C:H1'	2.50	0.47
6:G:81:LYS:HB3	6:G:82:LEU:H	1.49	0.47
20:U:46:LYS:O	20:U:48:ALA:N	2.47	0.47
24:W:16:LEU:HD12	24:W:20:GLU:HB2	1.95	0.47
17:2:35:LEU:O	17:2:37:VAL:HG13	2.15	0.47
1:A:2393:A:OP1	30:8:30:ARG:HB3	2.14	0.47
4:E:35:GLN:OE1	4:E:37:ARG:NH2	2.47	0.47
1:A:2065:C:H5''	1:A:2252:G:H1'	1.96	0.47
1:A:1094:U:C5'	1:A:1098:A:H61	2.27	0.47
1:A:2356:C:H4'	22:3:20:ARG:HG3	1.97	0.47
1:A:1728:G:O6	1:A:1730:U:H5'	2.14	0.47
30:8:37:SER:OG	30:8:39:LYS:O	2.29	0.47
21:V:68:PRO:HG2	21:V:91:LEU:O	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:539:G:H2'	1:A:540:G:H8	1.79	0.47
19:T:5:TYR:HB3	24:W:33:MET:HB2	1.95	0.47
11:O:79:ARG:CZ	11:O:109:GLY:HA3	2.45	0.47
1:A:5:A:H2'	1:A:6:A:C8	2.50	0.47
1:A:2635:C:H5''	4:E:77:ILE:O	2.15	0.47
1:A:257:A:H2'	1:A:258:G:O4'	2.15	0.47
5:F:37:VAL:HG21	11:O:6:LEU:HD21	1.97	0.47
1:A:196:A:N3	1:A:196:A:H2'	2.30	0.47
1:A:1219:G:H1	1:A:1230:C:H42	1.61	0.47
1:A:2032:G:H21	4:E:146:THR:HG23	1.80	0.47
10:N:50:GLY:O	10:N:53:LYS:NZ	2.41	0.47
26:4:36:CYS:O	26:4:36:CYS:SG	2.72	0.47
2:B:43:C:P	26:4:6:HIS:HE1	2.37	0.47
1:A:1114:G:H2'	1:A:1115:G:H8	1.78	0.47
13:O:78:LYS:O	13:O:82:GLU:HB3	2.15	0.47
1:A:2735:G:H1	1:A:2769:C:H42	1.62	0.47
11:O:146:VAL:HG22	11:O:147:LEU:HD23	1.96	0.47
6:G:143:GLU:O	26:4:28:LYS:NZ	2.36	0.47
1:A:1797:C:O2'	3:D:259:THR:OG1	2.25	0.47
1:A:1805:U:O2	3:D:50:THR:HB	2.15	0.47
1:A:1027:A:H8	1:A:1027:A:OP2	1.97	0.47
1:A:2153:G:C2	1:A:2154:G:C8	3.03	0.47
1:A:94:G:P	20:U:54:LYS:HE3	2.55	0.47
1:A:893:C:O2'	1:A:894:C:P	2.73	0.47
21:V:152:ALA:HB3	21:V:167:PRO:HA	1.97	0.47
1:A:2611:U:H2'	27:5:3:LYS:HZ2	1.79	0.47
1:A:2853:C:H2'	1:A:2854:G:H8	1.80	0.47
1:A:2030:A:H4'	1:A:2031:A:C8	2.50	0.47
17:2:66:ARG:HB2	17:2:88:ARG:HB3	1.97	0.47
16:1:109:LEU:HA	16:1:112:ARG:HG3	1.97	0.47
1:A:1716:U:O2'	1:A:1717:G:H5'	2.15	0.47
1:A:217:G:H2'	1:A:218:A:O4'	2.15	0.47
1:A:1842:G:O2'	3:D:253:GLN:OE1	2.32	0.47
4:E:60:ASN:HD22	4:E:63:LEU:CD2	2.15	0.47
4:E:37:ARG:HD2	4:E:44:TYR:OH	2.15	0.47
1:A:1090:U:N3	1:A:1102:C:N3	2.63	0.47
2:B:89:G:H2'	2:B:89(A):A:N3	2.30	0.47
1:A:2543:G:H2'	1:A:2544:G:C8	2.50	0.47
1:A:2793:G:C5	1:A:2794:C:C4	3.03	0.47
2:B:40:U:N3	2:B:43:C:H5''	2.30	0.47
1:A:2:G:N2	1:A:2901:C:N3	2.63	0.47
1:A:2012:G:OP1	18:S:11:ARG:NH2	2.43	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:Z:87:PRO:HA	23:Z:90:ILE:HG23	1.97	0.47
19:T:43:VAL:CG2	19:T:51:VAL:HG21	2.45	0.47
1:A:616:A:H8	5:F:176:LEU:HD11	1.80	0.47
1:A:184:C:H2'	1:A:185:U:H6	1.80	0.47
12:P:29:PHE:N	12:P:105:GLU:OE1	2.45	0.47
7:H:91:GLY:HA3	7:H:94:TYR:CE2	2.49	0.47
5:F:178:PRO:HB3	5:F:198:ALA:HB1	1.97	0.47
24:W:66:GLU:HG2	24:W:69:ARG:HH22	1.79	0.47
1:A:57:C:H2'	1:A:58:G:O4'	2.15	0.47
21:V:23:LYS:HE2	21:V:40:ASP:HB2	1.97	0.47
1:A:2161:C:H2'	1:A:2162:G:C8	2.50	0.46
1:A:1080:A:H62	1:A:1088:A:P	2.38	0.46
1:A:1019:U:O2'	1:A:1021:A:H2	1.98	0.46
1:A:2542:A:H1'	1:A:2543:G:N7	2.29	0.46
16:1:50:ARG:HG2	16:1:53:ARG:NH2	2.30	0.46
1:A:654(G):C:H2'	1:A:654(H):G:O4'	2.15	0.46
1:A:654(H):G:N1	1:A:654(I):C:N3	2.63	0.46
12:P:122:GLY:HA2	12:P:129:THR:HG21	1.97	0.46
1:A:669:G:O2'	1:A:670:A:P	2.73	0.46
13:0:70:LEU:O	13:0:72:ASP:N	2.46	0.46
12:P:69:PHE:HA	12:P:70:PRO:HD3	1.80	0.46
20:U:2:ARG:NH1	20:U:2:ARG:HA	2.31	0.46
11:O:60:MET:O	11:O:61:ARG:HD3	2.12	0.46
28:6:37:ARG:O	28:6:49:HIS:NE2	2.48	0.46
1:A:2112:G:H1	1:A:2169:A:N6	2.12	0.46
1:A:2156:G:H3'	1:A:2157:G:C8	2.49	0.46
1:A:1063:G:C5	1:A:1076:C:C2	3.03	0.46
21:V:30:ASN:ND2	21:V:90:VAL:O	2.47	0.46
21:V:10:ARG:HB3	21:V:36:LYS:HB3	1.98	0.46
15:R:24:PRO:O	15:R:94:ALA:HB2	2.15	0.46
1:A:1464:C:O2'	1:A:1528:A:H8	1.96	0.46
1:A:2233:U:H2'	1:A:2234:G:C8	2.51	0.46
15:R:16:ARG:HH12	15:R:83:ILE:HB	1.81	0.46
1:A:134:C:H42	1:A:145:G:H1	1.62	0.46
1:A:2346:A:N6	28:6:28:ARG:HH21	2.13	0.46
1:A:2129:C:O2'	1:A:2130:U:H5'	2.15	0.46
1:A:896:A:H3'	1:A:897:C:H5''	1.97	0.46
1:A:10:G:C5	1:A:2629:A:C6	3.03	0.46
21:V:54:HIS:HB3	21:V:101:PRO:HD3	1.96	0.46
1:A:2853:C:H2'	1:A:2854:G:C8	2.50	0.46
11:O:111:ARG:HG2	11:O:128:HIS:CD2	2.51	0.46
3:D:130:ALA:HA	3:D:192:THR:HA	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
21:V:70:LEU:HD23	21:V:70:LEU:HA	1.73	0.46
1:A:2572:A:N7	4:E:145:LYS:HB2	2.31	0.46
1:A:698:C:O2'	1:A:734:A:N6	2.47	0.46
1:A:1342:A:C2	1:A:1397:U:C2	3.03	0.46
1:A:213:A:H2'	1:A:214:G:O4'	2.15	0.46
8:K:117:GLU:HB2	8:K:118:LYS:H	1.51	0.46
1:A:495:G:N3	18:S:61:ASN:ND2	2.62	0.46
11:O:71:VAL:N	11:O:72:PRO:CD	2.78	0.46
11:O:59:LEU:O	11:O:61:ARG:N	2.48	0.46
1:A:2419:U:H5''	30:8:34:TRP:CD1	2.51	0.46
7:H:163:TYR:CE2	7:H:169:VAL:HG11	2.49	0.46
1:A:443:A:H1'	1:A:1201:C:O4'	2.15	0.46
14:Q:14:VAL:HG21	14:Q:89:ARG:HG2	1.97	0.46
6:G:41:GLN:NE2	6:G:60:LEU:HD12	2.31	0.46
1:A:2602:A:H4'	1:A:2603:G:C5'	2.46	0.46
21:V:105:VAL:HG13	21:V:106:GLY:H	1.79	0.46
1:A:616:A:C5	5:F:180:GLY:HA3	2.51	0.46
14:Q:104:GLY:O	14:Q:106:ARG:HG2	2.16	0.46
5:F:34:TRP:CE3	11:O:8:PRO:HB3	2.51	0.46
3:D:133:LEU:HB3	3:D:173:VAL:HG21	1.98	0.46
20:U:96:ILE:HD12	20:U:98:VAL:HG12	1.97	0.46
5:F:123:LEU:HA	5:F:192:LEU:HB3	1.97	0.46
1:A:1255:U:H5''	1:A:1256:G:H5''	1.96	0.46
4:E:72:VAL:O	4:E:73:GLU:O	2.33	0.46
1:A:2131:G:OP1	1:A:2132:U:H3'	2.16	0.46
4:E:47:VAL:HG22	4:E:48:GLN:N	2.30	0.46
1:A:881:G:H3'	1:A:882:G:H8	1.81	0.46
1:A:893:C:O2'	1:A:894:C:OP2	2.27	0.46
1:A:1094:U:H5'	1:A:1098:A:N1	2.31	0.46
2:B:55:U:O3'	6:G:27:ASN:ND2	2.48	0.46
27:5:3:LYS:HZ1	27:5:4:HIS:CE1	2.33	0.46
4:E:93:VAL:HG11	4:E:181:LEU:O	2.16	0.46
3:D:31:LYS:CE	3:D:33:LEU:HD12	2.46	0.46
1:A:1410:G:H2'	1:A:1411:C:C6	2.50	0.46
14:Q:107:GLU:H	14:Q:110:LEU:HD21	1.80	0.46
21:V:52:SER:OG	21:V:52:SER:O	2.29	0.46
1:A:1582:C:O2'	1:A:1586:A:H8	1.98	0.46
10:N:75:SER:OG	10:N:76:ALA:N	2.48	0.46
1:A:2402:C:H2'	1:A:2403:C:H5'	1.97	0.46
5:F:70:THR:HG23	5:F:72:ARG:H	1.79	0.46
1:A:1162:G:H21	17:2:89:GLN:HE22	1.64	0.46
17:2:14:VAL:HB	17:2:96:ILE:HG13	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:105:ILE:HA	3:D:105:ILE:HD13	1.82	0.46
10:N:68:GLU:OE2	10:N:78:ARG:NH1	2.49	0.46
1:A:242:G:H5''	30:8:62:LEU:HD13	1.98	0.46
1:A:2401:U:H3'	1:A:2402:C:C5'	2.45	0.46
1:A:2401:U:O2	1:A:2402:C:H5	1.99	0.46
1:A:581:C:H2'	1:A:582:G:C8	2.51	0.46
1:A:1783:A:H5'	1:A:2608:G:H4'	1.98	0.46
11:O:94:GLU:HG3	11:O:124:LYS:HD3	1.96	0.46
1:A:118:A:N3	1:A:178:G:H1'	2.31	0.46
4:E:67:PHE:CD2	4:E:69:LYS:HD3	2.51	0.46
1:A:2116:G:N1	1:A:2163:C:OP1	2.49	0.46
5:F:24:LEU:CB	5:F:25:PRO:CD	2.62	0.46
1:A:2291:U:O2'	1:A:2374:C:O2	2.27	0.46
2:B:87:G:H2'	2:B:89:G:N7	2.30	0.46
12:P:23:GLY:HA2	12:P:25:ASP:HB2	1.98	0.46
1:A:602:G:N2	1:A:655:A:N7	2.56	0.46
21:V:132:ASN:ND2	21:V:159:PRO:HB2	2.26	0.46
15:R:45:PHE:CE2	15:R:74:ARG:HD2	2.50	0.46
11:O:120:ALA:HB1	11:O:138:LEU:HB3	1.97	0.46
1:A:2530:A:C4	7:H:157:TYR:HE2	2.33	0.46
1:A:1262:A:N3	27:5:10:LYS:HE3	2.31	0.46
1:A:2786:U:O2	4:E:62:PRO:HB3	2.15	0.46
1:A:2129:C:H2'	1:A:2130:U:O4'	2.15	0.46
20:U:54:LYS:O	20:U:55:TYR:HB3	2.15	0.46
4:E:46:ALA:HB2	4:E:82:ARG:HA	1.96	0.46
1:A:882:G:H1	1:A:894:C:N4	2.14	0.46
1:A:2795:G:H1'	1:A:2802:G:C6	2.51	0.46
1:A:782:A:H4'	1:A:783:A:H5'	1.98	0.46
2:B:15:A:H1'	2:B:109:G:N9	2.31	0.46
1:A:2:G:H22	1:A:2901:C:H42	1.64	0.46
1:A:2387:U:H1'	22:3:41:ARG:HD2	1.98	0.46
1:A:1186:G:H8	1:A:1186:G:O5'	1.99	0.46
1:A:108:U:H2'	1:A:109:G:C8	2.51	0.46
24:W:62:THR:O	24:W:66:GLU:HG3	2.16	0.46
1:A:577:G:O2'	1:A:1254:A:OP1	2.33	0.46
13:O:115:GLU:OE2	27:5:55:ARG:HB2	2.16	0.46
1:A:2685:G:O2'	1:A:2726:U:H5	1.99	0.46
1:A:397:G:O2'	1:A:2231:C:H1'	2.16	0.46
11:O:59:LEU:HG	30:8:56:GLU:OE2	2.16	0.46
1:A:2128:C:H2'	1:A:2129:C:C1'	2.45	0.46
1:A:547:A:H3'	1:A:548:A:C8	2.50	0.46
1:A:662:G:OP1	11:O:15:ARG:NE	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:Z:87:PRO:O	23:Z:89:GLU:N	2.49	0.46
1:A:2402:C:OP1	1:A:2402:C:H4'	2.15	0.46
1:A:2355:C:O2	22:3:39:ARG:NH2	2.49	0.46
1:A:2880:C:O2'	13:0:90:ARG:NH1	2.40	0.46
23:Z:81:LYS:HZ2	23:Z:82:LEU:HB3	1.81	0.46
1:A:2833:G:O2'	1:A:2834:G:OP1	2.25	0.46
1:A:673:C:H5''	5:F:81:PRO:HD2	1.97	0.46
1:A:2773:C:P	4:E:166:THR:HG1	2.39	0.46
11:O:71:VAL:H	11:O:72:PRO:HD2	1.80	0.45
4:E:74:PRO:O	4:E:75:VAL:C	2.55	0.45
1:A:1083:U:O2	1:A:1085:A:H2'	2.16	0.45
1:A:2802:G:C6	1:A:2803:C:C2	3.04	0.45
2:B:42:C:H4'	6:G:67:LYS:HD2	1.96	0.45
7:H:20:ALA:HB1	7:H:23:ARG:HH21	1.82	0.45
1:A:173:G:C2	1:A:174:C:C2	3.04	0.45
17:2:76:LYS:HD2	17:2:80:GLN:O	2.16	0.45
23:Z:81:LYS:NZ	23:Z:82:LEU:HB3	2.31	0.45
12:P:37:LEU:HD21	12:P:130:LYS:HB3	1.98	0.45
1:A:171:G:H2'	1:A:172:C:H6	1.81	0.45
1:A:769:G:H2'	1:A:770:G:C8	2.51	0.45
1:A:901:A:N3	1:A:901:A:H2'	2.30	0.45
1:A:1511:A:H2'	1:A:1512:G:O4'	2.15	0.45
1:A:270(B):A:H62	1:A:270(X):G:N2	2.13	0.45
1:A:828:U:H4'	1:A:831:G:N1	2.30	0.45
1:A:482:A:OP2	1:A:507:A:N6	2.37	0.45
9:M:112:LEU:HA	9:M:112:LEU:HD12	1.75	0.45
1:A:2052:G:O4'	4:E:142:GLY:HA3	2.15	0.45
1:A:389:G:OP1	23:Z:25:LYS:HD2	2.16	0.45
1:A:2168:G:H2'	1:A:2168:G:N3	2.31	0.45
1:A:2646:C:OP2	1:A:2732:G:O2'	2.20	0.45
1:A:1171:G:N2	1:A:1173:G:O2'	2.49	0.45
16:1:66:ASN:HB2	16:1:76:TYR:HB2	1.98	0.45
17:2:2:PHE:O	17:2:42:GLY:N	2.41	0.45
2:B:11:C:H3'	2:B:12:C:C6	2.51	0.45
21:V:16:SER:HA	21:V:19:ARG:HD2	1.98	0.45
7:H:144:VAL:O	7:H:148:ILE:HG12	2.16	0.45
1:A:1851:U:H2'	1:A:1852:C:O4'	2.16	0.45
11:O:47:ASP:HB3	11:O:48:PRO:O	2.15	0.45
1:A:2131:G:H5'	1:A:2132:U:H5''	1.98	0.45
20:U:52:SER:OG	20:U:56:PRO:CG	2.54	0.45
1:A:2294:C:OP2	14:Q:13:ARG:NH1	2.48	0.45
1:A:242:G:H5'	30:8:62:LEU:HD13	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
24:W:31:GLU:HB2	24:W:53:LEU:HD11	1.98	0.45
20:U:81:LYS:HD3	20:U:97:ARG:NH2	2.31	0.45
1:A:1601:G:O2'	29:7:49:ARG:NH2	2.47	0.45
21:V:63:ASP:HB3	21:V:65:GLN:HG3	1.99	0.45
12:P:118:LEU:HB2	12:P:131:ILE:HD13	1.97	0.45
1:A:2027:G:H2'	1:A:2028:U:O4'	2.15	0.45
8:K:90:GLY:O	8:K:121:LYS:HG2	2.16	0.45
28:6:44:ARG:HG3	28:6:45:LYS:H	1.81	0.45
1:A:2065:C:H2'	1:A:2066:C:H6	1.79	0.45
1:A:2542:A:O2'	1:A:2543:G:C8	2.67	0.45
1:A:1040:C:H2'	1:A:1041:C:C6	2.51	0.45
20:U:84:ARG:HB3	20:U:95:LYS:HG3	1.97	0.45
16:1:75:ASN:HD22	16:1:78:THR:CG2	2.30	0.45
1:A:1416:G:H2'	1:A:1417:C:C6	2.51	0.45
5:F:125:LEU:HD12	5:F:196:LEU:HD22	1.99	0.45
1:A:2186:G:C2	1:A:2187:G:C8	3.05	0.45
15:R:51:ARG:HG2	15:R:98:LYS:HE3	1.99	0.45
3:D:182:LEU:O	3:D:271:ILE:HG12	2.17	0.45
1:A:1823:G:P	3:D:54:ARG:HH21	2.40	0.45
1:A:388:G:OP1	23:Z:32:LYS:N	2.49	0.45
3:D:35:LYS:HZ1	3:D:64:ILE:CG1	2.23	0.45
1:A:289:A:H5'	1:A:290:G:OP2	2.17	0.45
1:A:270(R):G:H2'	1:A:270(S):G:C8	2.52	0.45
1:A:2883:A:H3'	1:A:2884:U:H5'	1.98	0.45
17:2:62:LEU:HD21	17:2:95:LEU:HB2	1.98	0.45
24:W:33:MET:HG2	24:W:37:PHE:CE1	2.52	0.45
1:A:637:A:P	11:O:116:GLY:H	2.39	0.45
1:A:363:G:C6	1:A:363(A):A:C5	3.05	0.45
7:H:45:VAL:HA	7:H:50:VAL:HA	1.98	0.45
1:A:565:C:H4'	1:A:1253:A:N6	2.31	0.45
1:A:1628:G:H2'	1:A:1629:U:C6	2.51	0.45
7:H:18:GLU:HB2	7:H:25:LYS:HD2	1.98	0.45
4:E:50:GLY:HA2	4:E:78:LEU:HD22	1.99	0.45
1:A:2542:A:HO2'	1:A:2543:G:P	2.39	0.45
1:A:2472:G:N1	1:A:2477:C:OP1	2.50	0.45
14:Q:83:LYS:HB3	14:Q:109:GLY:N	2.32	0.45
6:G:122:PRO:HB3	6:G:170:ARG:HH11	1.81	0.45
1:A:142:G:H2'	1:A:143:C:C6	2.52	0.45
21:V:23:LYS:HA	21:V:23:LYS:HD3	1.80	0.45
1:A:954:G:O2'	1:A:2274:A:N1	2.47	0.45
30:8:52:LYS:HG2	30:8:52:LYS:H	1.51	0.45
4:E:103:ASP:N	4:E:200:GLU:O	2.45	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:832:G:H5'	11:O:45:LEU:HD11	1.97	0.45
1:A:2113:U:OP1	1:A:2118:U:H5'	2.16	0.45
5:F:64:ILE:O	5:F:65:TRP:CD1	2.69	0.45
2:B:1(M):A:N6	2:B:117:G:O6	2.50	0.45
1:A:833:U:H2'	1:A:834:C:C6	2.52	0.45
1:A:2659:G:OP1	7:H:158:HIS:NE2	2.50	0.45
1:A:1171:G:N1	1:A:1174:A:N1	2.64	0.45
4:E:101:ARG:HD3	4:E:171:GLU:HA	1.99	0.45
25:X:19:GLN:HE22	25:X:52:HIS:HE1	1.63	0.45
22:3:70:GLN:OE1	22:3:72:ARG:HD2	2.17	0.45
1:A:1798:U:H5'	3:D:259:THR:OG1	2.16	0.45
1:A:1017:G:H1	1:A:1145:C:H42	1.64	0.45
1:A:2008:C:H2'	1:A:2009:G:H8	1.81	0.45
1:A:1028:A:N6	1:A:1125:G:H2'	2.32	0.45
1:A:996:A:O4'	16:1:92:ARG:NH2	2.50	0.45
11:O:49:ARG:HG3	30:8:55:ALA:O	2.16	0.45
2:B:40:U:H3'	2:B:41:U:H5'	1.99	0.45
1:A:2516:G:C6	1:A:2517:C:N4	2.85	0.45
1:A:654(C):G:H2'	1:A:654(D):G:O4'	2.16	0.45
1:A:2864:G:OP1	15:R:119:LYS:HD2	2.16	0.45
1:A:270(V):G:H2'	1:A:270(W):G:H8	1.81	0.45
1:A:2593:U:H2'	1:A:2594:C:C6	2.52	0.45
1:A:929:G:H8	1:A:929:G:O5'	2.00	0.45
1:A:1758:G:N3	1:A:1758:G:H5''	2.31	0.45
4:E:11:MET:CB	4:E:24:THR:HA	2.45	0.45
1:A:1210:A:H5'	1:A:1212:G:H5'	1.99	0.45
1:A:676:A:H8	1:A:2069:G:N2	2.01	0.45
1:A:1039:G:N1	1:A:1116:C:N3	2.52	0.45
4:E:175:VAL:HG22	4:E:177:PRO:HD3	1.98	0.45
15:R:116:ALA:HB1	15:R:121:ILE:HD11	1.99	0.45
17:2:76:LYS:HZ1	17:2:82:ARG:HH11	1.65	0.45
1:A:2688:U:C5	1:A:2720:U:OP2	2.69	0.45
1:A:2694:G:O2'	1:A:2695:C:H5'	2.17	0.45
24:W:24:LEU:O	24:W:28:LYS:HG2	2.16	0.45
1:A:1655:A:H4'	4:E:115:GLY:N	2.32	0.45
1:A:910:A:C5	12:P:13:GLN:HG3	2.51	0.45
4:E:41:LYS:HE3	4:E:41:LYS:HB2	1.75	0.45
1:A:2376:A:OP1	1:A:2376:A:H8	2.00	0.45
23:Z:46:LEU:HD12	23:Z:46:LEU:HA	1.85	0.45
1:A:2115:G:H3'	1:A:2115:G:OP2	2.16	0.45
4:E:21:VAL:HG13	4:E:22:PRO:HD2	1.97	0.45
21:V:151:HIS:N	21:V:154:ASP:OD2	2.49	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:639:U:H2'	1:A:640:C:C6	2.51	0.45
1:A:1006:C:C2	1:A:1138:G:N2	2.85	0.45
5:F:170:LEU:HA	5:F:171:PRO:HD2	1.85	0.45
8:K:111:PRO:C	8:K:113:ARG:H	2.20	0.45
8:K:8:PRO:HD3	8:K:15:VAL:HG22	1.98	0.45
10:N:70:LYS:NZ	10:N:70:LYS:HB3	2.32	0.45
26:4:15:ILE:H	26:4:15:ILE:HG13	1.46	0.45
1:A:1396:U:H2'	1:A:1396:U:O2	2.17	0.45
11:O:36:LYS:HZ3	11:O:36:LYS:HG2	1.67	0.45
28:6:28:ARG:HD3	28:6:28:ARG:HA	1.84	0.44
5:F:67:GLN:HB2	5:F:67:GLN:HE21	1.60	0.44
1:A:1054:A:OP2	1:A:1054:A:H8	2.00	0.44
1:A:1052:C:C2	1:A:1107:G:N2	2.85	0.44
1:A:307:G:N2	1:A:309:G:H3'	2.32	0.44
7:H:131:VAL:HG12	7:H:132:ARG:O	2.17	0.44
1:A:1110:G:H2'	1:A:1111:A:C8	2.52	0.44
1:A:83:G:N1	1:A:102:G:H2'	2.32	0.44
1:A:2321:G:N3	1:A:2321:G:H2'	2.32	0.44
1:A:1729:A:O2'	1:A:1730:U:H5''	2.17	0.44
1:A:270(R):G:H2'	1:A:270(S):G:H8	1.80	0.44
1:A:2105:C:H2'	1:A:2106:G:H8	1.83	0.44
1:A:1416:G:O2'	1:A:1417:C:O5'	2.29	0.44
1:A:1540:G:C2	1:A:1541:U:C2	3.05	0.44
4:E:101:ARG:O	4:E:201:THR:OG1	2.35	0.44
1:A:601:C:H4'	5:F:104:LYS:HZ3	1.82	0.44
30:8:52:LYS:HB3	30:8:52:LYS:HE2	1.78	0.44
24:W:4:SER:HB3	24:W:5:GLU:OE2	2.16	0.44
1:A:1441:G:H2'	1:A:1442:G:H8	1.82	0.44
1:A:1270:C:H5''	1:A:1271:G:O5'	2.17	0.44
8:K:131:LYS:HB3	8:K:132:PRO:HA	1.99	0.44
9:M:6:PRO:HB3	9:M:41:ASP:OD1	2.17	0.44
8:K:92:VAL:HG23	8:K:96:ASP:HB2	1.99	0.44
8:K:79:ILE:HB	8:K:142:VAL:HB	1.98	0.44
9:M:69:GLN:O	9:M:71:ILE:HG23	2.17	0.44
1:A:2776:A:OP1	1:A:2776:A:H3'	2.17	0.44
1:A:2750:A:OP2	7:H:62:LYS:NZ	2.40	0.44
14:Q:19:LYS:O	14:Q:21:THR:HG22	2.18	0.44
9:M:95:PRO:O	9:M:98:VAL:HG22	2.18	0.44
10:N:87:ILE:HG23	10:N:88:ASN:O	2.17	0.44
1:A:1011:G:C2	1:A:1151:G:C2	3.05	0.44
1:A:1614:A:C6	18:S:91:GLY:HA2	2.52	0.44
4:E:116:VAL:C	4:E:118:LYS:H	2.19	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
15:R:91:ARG:NH1	15:R:124:ASP:OD1	2.47	0.44
25:X:22:ALA:O	25:X:26:LEU:HG	2.17	0.44
16:1:65:ILE:O	16:1:68:ALA:N	2.50	0.44
4:E:2:LYS:NZ	4:E:95:ILE:O	2.50	0.44
26:4:31:ILE:HG22	26:4:32:TYR:HB2	1.98	0.44
1:A:2016:U:H1'	27:5:6:VAL:HG13	1.99	0.44
1:A:1276:A:O2'	13:0:12:ARG:NH2	2.48	0.44
10:N:25:LEU:HB2	10:N:38:VAL:HG23	1.98	0.44
9:M:67:LEU:HA	9:M:87:LEU:HB3	1.98	0.44
1:A:528:A:C2	1:A:2042:A:H2'	2.52	0.44
16:1:91:ASP:O	16:1:92:ARG:HG2	2.17	0.44
1:A:2658:C:O3'	7:H:158:HIS:NE2	2.51	0.44
1:A:636:G:OP2	11:O:113:LYS:NZ	2.37	0.44
1:A:649:G:H2'	1:A:650:C:O4'	2.17	0.44
21:V:100:VAL:HG13	21:V:101:PRO:HD2	1.99	0.44
11:O:65:ARG:HH22	30:8:47:LYS:HE2	1.82	0.44
7:H:97:ARG:O	7:H:99:VAL:N	2.49	0.44
1:A:2017:U:O2	27:5:10:LYS:HB2	2.17	0.44
9:M:14:VAL:HA	9:M:135:PRO:HD2	1.98	0.44
1:A:2474:C:H5''	1:A:2475:C:C5	2.53	0.44
1:A:977:G:N3	1:A:1001:A:H2	2.16	0.44
1:A:126:A:O5'	29:7:19:ARG:HG3	2.18	0.44
1:A:895:U:H5'	21:V:146:ILE:HG12	1.98	0.44
1:A:1063:G:H1	1:A:1064:C:HO2'	1.63	0.44
1:A:2756:U:H4'	1:A:2757:A:OP1	2.17	0.44
1:A:2543:G:H21	1:A:2646:C:H5''	1.82	0.44
1:A:2851:A:O2'	13:0:64:ARG:NH2	2.50	0.44
1:A:1292:U:H2'	1:A:1293:C:C6	2.52	0.44
6:G:20:ILE:O	6:G:20:ILE:HG13	2.16	0.44
3:D:97:TYR:HB2	3:D:101:GLU:O	2.17	0.44
3:D:13:ARG:HD2	3:D:16:MET:HE3	2.00	0.44
3:D:109:ASP:O	3:D:111:LEU:N	2.51	0.44
1:A:686:G:H21	1:A:788:A:H61	1.65	0.44
30:8:52:LYS:C	30:8:54:GLU:H	2.21	0.44
1:A:588:U:H1'	5:F:90:PHE:CG	2.53	0.44
1:A:78:A:H2'	1:A:79:G:H8	1.82	0.44
5:F:129:PHE:HA	5:F:142:TRP:NE1	2.32	0.44
7:H:27:LYS:HB2	7:H:32:GLU:HB3	1.98	0.44
4:E:8:LYS:O	4:E:10:GLY:N	2.51	0.44
4:E:11:MET:HG3	4:E:24:THR:CA	2.48	0.44
4:E:25:VAL:CG1	4:E:26:ILE:N	2.80	0.44
1:A:2134:A:H2'	1:A:2134:A:N3	2.33	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1093:G:N7	1:A:1094:U:C4	2.86	0.44
3:D:43:ARG:HH11	3:D:44:ASN:ND2	2.14	0.44
1:A:2850:A:C2	1:A:2851:A:C4	3.05	0.44
4:E:101:ARG:CZ	4:E:171:GLU:HB2	2.46	0.44
1:A:2110:G:H5''	1:A:2145:C:H42	1.82	0.44
1:A:2148:G:H2'	1:A:2149:G:H8	1.82	0.44
22:3:50:ASN:ND2	22:3:81:VAL:O	2.38	0.44
12:P:110:THR:OG1	12:P:113:GLN:N	2.48	0.44
1:A:435:C:H2'	1:A:436:C:H5'	1.99	0.44
7:H:87:LEU:HD23	7:H:164:TYR:HA	1.99	0.44
1:A:19:C:OP2	16:1:30:LYS:NZ	2.48	0.44
28:6:15:GLU:CB	28:6:47:THR:CG2	2.95	0.44
5:F:68:LYS:HB3	5:F:69:HIS:H	1.68	0.44
1:A:1106:G:N2	1:A:1107:G:N3	2.66	0.44
1:A:1332:G:N2	1:A:1610:A:C8	2.86	0.44
4:E:203:LYS:O	4:E:204:ALA:HB3	2.18	0.44
1:A:2145:C:H6	1:A:2147:G:N2	2.15	0.44
1:A:2572:A:OP1	1:A:2574:G:H4'	2.17	0.44
12:P:63:LYS:HB2	21:V:116:VAL:HG11	1.99	0.44
1:A:26:G:C6	1:A:27:G:N1	2.85	0.44
1:A:118:A:H1'	1:A:178:G:O4'	2.18	0.44
9:M:112:LEU:O	9:M:115:ARG:N	2.50	0.44
1:A:2257:U:O2'	1:A:2258:C:H5'	2.17	0.44
1:A:2176:A:H2'	1:A:2177:C:H6	1.82	0.44
1:A:1239:G:H2'	1:A:1240:U:O4'	2.17	0.44
14:Q:49:VAL:HG21	14:Q:77:ALA:HB2	1.98	0.44
1:A:2207:C:H42	1:A:2217:G:H1	1.64	0.44
1:A:476:G:H4'	1:A:502:A:N1	2.33	0.44
4:E:55:ASN:HD21	4:E:75:VAL:N	2.15	0.44
1:A:2115:G:C6	1:A:2117:A:C8	3.06	0.44
4:E:21:VAL:CG1	4:E:22:PRO:N	2.80	0.44
1:A:523:C:O2'	1:A:553:U:O2	2.35	0.44
1:A:2015:A:N3	27:5:2:ALA:N	2.65	0.44
1:A:1131:G:O6	1:A:2024:G:N2	2.43	0.44
27:5:25:LEU:HD23	27:5:25:LEU:HA	1.66	0.44
1:A:128:C:H4'	1:A:129:C:OP1	2.18	0.44
5:F:157:VAL:HG12	5:F:198:ALA:HB1	2.00	0.44
20:U:97:ARG:NH2	20:U:98:VAL:HB	2.33	0.44
1:A:78:A:H2'	1:A:79:G:C8	2.53	0.44
21:V:3:TYR:O	21:V:57:ILE:HA	2.18	0.44
9:M:66:LYS:O	9:M:70:LYS:N	2.50	0.44
18:S:111:HIS:CG	18:S:113:LYS:HZ1	2.36	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:205:G:O2'	1:A:206:U:OP2	2.36	0.44
1:A:2168:G:N2	1:A:2169:A:H3'	2.33	0.44
7:H:7:LEU:HG	7:H:7:LEU:H	1.63	0.44
1:A:1010:A:H5'	16:1:62:ILE:HG21	2.00	0.44
3:D:31:LYS:HZ3	3:D:94:LEU:HD11	1.80	0.44
1:A:2295:C:OP2	14:Q:10:ARG:HD3	2.18	0.44
14:Q:25:ARG:HH12	14:Q:42:ASP:CG	2.21	0.44
1:A:271:G:H2'	1:A:272:G:H8	1.81	0.44
1:A:2693:A:H2'	1:A:2694:G:H8	1.83	0.44
19:T:25:LYS:HA	19:T:81:VAL:O	2.18	0.44
1:A:479:A:N3	1:A:481:G:H5''	2.33	0.44
28:6:25:LYS:HE2	28:6:27:LYS:HZ2	1.82	0.44
4:E:50:GLY:HA3	4:E:74:PRO:HG3	2.00	0.44
1:A:2156:G:C6	1:A:2157:G:N1	2.86	0.44
1:A:883:G:O2'	1:A:884:C:H5'	2.18	0.44
1:A:1053:C:N4	1:A:1106:G:C6	2.86	0.44
1:A:84:A:H3'	20:U:8:LYS:HG2	2.00	0.44
2:B:24:G:H4'	2:B:25:A:H8	1.82	0.44
1:A:1517:G:H4'	1:A:1556:C:O2'	2.16	0.44
3:D:92:ILE:HD12	3:D:104:TYR:CD2	2.52	0.44
21:V:26:GLY:HA2	21:V:86:VAL:H	1.82	0.44
1:A:1151:G:H4'	16:1:81:HIS:CG	2.53	0.44
1:A:1869:G:H2'	1:A:1871:A:N7	2.33	0.44
20:U:67:LEU:HA	20:U:67:LEU:HD12	1.62	0.44
1:A:1550:C:OP1	1:A:1727:U:O2'	2.17	0.44
22:3:19:LYS:HA	22:3:19:LYS:HD3	1.83	0.44
10:N:24:VAL:HA	10:N:39:ILE:HG22	2.00	0.44
1:A:2685:G:P	15:R:51:ARG:HH22	2.41	0.44
1:A:2537:U:H2'	1:A:2538:C:C6	2.53	0.44
10:N:65:THR:O	10:N:79:PHE:HB2	2.18	0.44
8:K:64:GLU:HA	8:K:67:ARG:HB2	2.00	0.44
1:A:657:U:H2'	1:A:658:C:C6	2.52	0.44
1:A:843:G:H1	1:A:935:C:H42	1.66	0.44
10:N:44:LYS:HA	10:N:44:LYS:HD3	1.79	0.44
1:A:2344:U:O2'	28:6:37:ARG:HG2	2.18	0.43
1:A:896:A:N3	21:V:176:PRO:HG2	2.33	0.43
1:A:2755:C:O2'	1:A:2756:U:H2'	2.18	0.43
1:A:1112:G:O3'	7:H:3:ARG:HA	2.18	0.43
1:A:1800:C:H3'	3:D:147:LEU:HD23	2.00	0.43
1:A:2795:G:H2'	1:A:2798:C:P	2.58	0.43
1:A:2294:C:P	14:Q:89:ARG:HH12	2.40	0.43
14:Q:88:ASP:OD1	14:Q:89:ARG:N	2.44	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1592:C:H2'	1:A:1593:G:C8	2.53	0.43
1:A:2143:C:H2'	1:A:2144:U:C6	2.53	0.43
1:A:2710:C:OP1	13:0:15:SER:HB3	2.18	0.43
1:A:459:U:H2'	1:A:460:A:H8	1.83	0.43
15:R:19:LEU:HD22	15:R:86:ILE:HG22	2.00	0.43
1:A:90:U:O2	1:A:90:U:H3'	2.18	0.43
1:A:239:U:H2'	1:A:240:G:O4'	2.18	0.43
1:A:1955:U:O3'	1:A:1956:U:H6	2.02	0.43
1:A:456:C:O2'	1:A:457:A:H5'	2.17	0.43
1:A:2224:G:OP1	3:D:268:ARG:NH1	2.51	0.43
1:A:1071:G:N7	1:A:1097:U:H4'	2.33	0.43
1:A:1110:G:O5'	1:A:1110:G:H8	2.00	0.43
1:A:2748:A:C8	1:A:2753:A:N6	2.86	0.43
3:D:23:GLU:O	3:D:25:THR:N	2.51	0.43
3:D:31:LYS:HB2	3:D:31:LYS:HE3	1.83	0.43
1:A:2294:C:H5'	14:Q:10:ARG:HD2	2.00	0.43
15:R:107:ASP:HB2	15:R:108:ARG:H	1.59	0.43
1:A:2148:G:H2'	1:A:2149:G:C8	2.53	0.43
2:B:39:A:N1	26:4:1:MET:N	2.61	0.43
8:K:109:ILE:HB	8:K:130:TYR:OH	2.18	0.43
1:A:265:A:H1'	1:A:266:G:O4'	2.18	0.43
24:W:10:LEU:HD12	24:W:10:LEU:HA	1.86	0.43
1:A:1314:C:H42	1:A:1338:G:H1	1.65	0.43
16:1:25:TRP:C	16:1:25:TRP:CD1	2.92	0.43
5:F:152:GLU:OE1	5:F:191:ARG:HD2	2.18	0.43
16:1:8:VAL:HG12	16:1:11:ARG:HH21	1.82	0.43
1:A:919:G:N2	1:A:2269:A:OP2	2.51	0.43
10:N:98:VAL:HG22	10:N:117:LEU:HB3	2.01	0.43
4:E:63:LEU:O	4:E:73:GLU:OE1	2.36	0.43
4:E:36:ARG:NH2	4:E:88:GLY:HA2	2.33	0.43
1:A:880:G:H2'	1:A:881:G:H8	1.82	0.43
1:A:892:G:C5	1:A:893:C:N4	2.86	0.43
1:A:1061:U:O3'	1:A:1070:A:H4'	2.18	0.43
1:A:1651:G:OP1	13:0:37:THR:HG21	2.19	0.43
9:M:56:ASN:H	9:M:125:GLY:CA	2.27	0.43
1:A:2317:C:H2'	1:A:2318:G:O4'	2.18	0.43
1:A:39:C:H2'	1:A:40:C:C6	2.53	0.43
1:A:1416:G:H2'	1:A:1417:C:H6	1.83	0.43
1:A:1688:U:H1'	1:A:1701:A:C6	2.54	0.43
16:1:17:ILE:HG23	16:1:39:LEU:HD12	2.00	0.43
1:A:2840:C:H4'	13:0:53:HIS:CE1	2.54	0.43
5:F:155:LEU:HD22	5:F:186:ILE:HA	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1324:G:H4'	1:A:1616:A:C2	2.53	0.43
1:A:193:U:O3'	1:A:803:U:H4'	2.18	0.43
1:A:138:G:N2	19:T:44:GLU:OE2	2.44	0.43
5:F:63:LYS:HZ1	5:F:67:GLN:NE2	2.08	0.43
1:A:1055:G:N3	1:A:1085:A:H2	2.16	0.43
1:A:307:G:N1	1:A:310:A:OP2	2.51	0.43
30:8:29:LYS:O	30:8:31:HIS:N	2.51	0.43
1:A:2420:C:OP1	30:8:34:TRP:CE3	2.72	0.43
1:A:1436:G:H1'	1:A:1477:A:O2'	2.19	0.43
12:P:23:GLY:HA2	12:P:24:GLY:HA3	1.63	0.43
1:A:1491:G:O2'	3:D:101:GLU:HB2	2.18	0.43
1:A:1819:A:OP1	3:D:161:THR:HG21	2.18	0.43
1:A:2735:G:H2'	1:A:2736:G:C8	2.52	0.43
10:N:114:ILE:O	10:N:118:ALA:N	2.49	0.43
6:G:25:TYR:OH	6:G:168:GLU:OE2	2.34	0.43
1:A:1275:A:N1	1:A:1295:C:O2'	2.47	0.43
1:A:2773:C:OP1	4:E:166:THR:OG1	2.36	0.43
1:A:1790:C:H2'	1:A:1791:A:C5	2.54	0.43
3:D:159:ALA:HB1	3:D:198:ASN:O	2.18	0.43
29:7:34:ARG:NH1	29:7:41:ARG:O	2.51	0.43
26:4:39:CYS:C	26:4:41:PRO:HD2	2.32	0.43
6:G:112:PRO:HB2	26:4:35:VAL:CG1	2.48	0.43
1:A:1051:G:H2'	1:A:1052:C:H5'	2.01	0.43
2:B:3:C:N4	2:B:117:G:H1	2.02	0.43
30:8:29:LYS:HB2	30:8:44:LYS:CB	2.42	0.43
5:F:53:THR:HG22	5:F:56:GLU:CG	2.48	0.43
1:A:2191:G:C4	1:A:2192:G:C8	3.06	0.43
2:B:12:C:H6	2:B:12:C:OP2	2.01	0.43
6:G:174:GLU:OE1	6:G:182:LYS:NZ	2.41	0.43
1:A:254:G:H4'	1:A:384:U:H5'	1.99	0.43
1:A:856:C:O2'	1:A:857:C:OP1	2.23	0.43
18:S:111:HIS:HB2	18:S:112:GLY:H	1.61	0.43
12:P:31:ASP:O	12:P:134:ARG:HB3	2.19	0.43
11:O:46:LYS:HD3	11:O:51:PHE:CG	2.54	0.43
1:A:1084:A:O2'	1:A:1105:U:H1'	2.19	0.43
1:A:1094:U:O2'	1:A:1095:A:H5''	2.19	0.43
1:A:2749:A:O3'	7:H:62:LYS:HE2	2.18	0.43
1:A:226:G:H21	1:A:228:A:H62	1.66	0.43
1:A:1339:G:H21	1:A:1603:A:H1'	1.83	0.43
24:W:37:PHE:O	24:W:41:ILE:HG23	2.19	0.43
4:E:116:VAL:HG23	4:E:120:TRP:HD1	1.83	0.43
1:A:152:G:H2'	1:A:153:C:O4'	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:686:G:H2'	1:A:788:A:N1	2.34	0.43
6:G:123:ASN:C	6:G:125:PHE:H	2.22	0.43
14:Q:5:THR:OG1	14:Q:7:TYR:HB3	2.19	0.43
1:A:343:C:H2'	1:A:344:G:C8	2.53	0.43
1:A:2224:G:H4'	1:A:2226:C:C2	2.53	0.43
28:6:11:LEU:HD23	28:6:51:GLU:OE1	2.18	0.43
3:D:67:PHE:HB3	3:D:153:ALA:HB3	1.99	0.43
1:A:1579:A:H2'	1:A:1580:A:C8	2.53	0.43
1:A:579:G:H2'	1:A:580:C:C6	2.54	0.43
1:A:2784:C:H4'	4:E:42:ASP:OD1	2.18	0.43
1:A:2419:U:H3'	30:8:34:TRP:NE1	2.34	0.43
7:H:83:TYR:OH	7:H:132:ARG:NH2	2.51	0.43
1:A:1112:G:H5'	7:H:3:ARG:NE	2.34	0.43
2:B:48:A:H4'	14:Q:95:HIS:CD2	2.45	0.43
1:A:814:C:H5''	17:2:84:LYS:HB3	2.00	0.43
1:A:1525:G:H2'	1:A:1526:G:H8	1.84	0.43
15:R:26:ASP:O	15:R:49:VAL:HG12	2.18	0.43
5:F:120:GLU:HG3	5:F:122:LYS:HG2	2.00	0.43
3:D:37:LEU:O	3:D:38:LYS:C	2.57	0.43
21:V:108:PRO:HB3	21:V:144:LEU:HD11	2.00	0.43
1:A:856:C:H3'	1:A:856:C:C6	2.53	0.43
1:A:1484:G:C2	1:A:1506:C:C2	3.07	0.43
1:A:2615:U:C2	27:5:7:PRO:HA	2.53	0.43
1:A:2623:G:H2'	1:A:2624:G:C8	2.54	0.43
1:A:2556:C:H2'	1:A:2557:G:O4'	2.19	0.43
1:A:1810:A:H2'	1:A:1811:G:O4'	2.19	0.43
5:F:200:GLU:OE2	5:F:201:VAL:N	2.52	0.43
10:N:2:ILE:HD12	10:N:6:THR:HG21	1.99	0.43
1:A:2115:G:C6	1:A:2117:A:H8	2.36	0.43
1:A:2129:C:C2'	1:A:2130:U:H5'	2.49	0.43
1:A:2130:U:O2'	1:A:2134:A:H8	2.01	0.43
1:A:2157:G:H2'	1:A:2158:A:H8	1.84	0.43
9:M:56:ASN:HB3	9:M:59:LYS:HB2	2.00	0.43
1:A:783:A:C8	1:A:784:A:H4'	2.49	0.43
1:A:2:G:H1	1:A:2901:C:N4	2.10	0.43
14:Q:110:LEU:HB2	14:Q:112:PHE:CZ	2.54	0.43
1:A:640:C:H42	1:A:648:G:H1	1.67	0.43
8:K:74:ASN:HB2	8:K:75:LEU:H	1.51	0.43
6:G:170:ARG:NH2	6:G:174:GLU:OE1	2.37	0.43
20:U:46:LYS:HB2	20:U:46:LYS:HE3	1.28	0.43
1:A:184:C:H2'	1:A:185:U:C6	2.54	0.43
1:A:270(E):G:H2'	1:A:270(F):U:O4'	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:588:U:H2'	1:A:589:C:C6	2.54	0.43
17:2:44:LYS:O	17:2:46:VAL:HG12	2.19	0.43
8:K:10:GLU:OE2	8:K:11:ASN:ND2	2.52	0.43
23:Z:53:VAL:HG22	23:Z:74:VAL:HG13	2.00	0.43
1:A:988:A:P	25:X:11:SER:HB2	2.59	0.43
1:A:2477:C:H5'	1:A:2479:G:O6	2.19	0.43
1:A:2516:G:C6	1:A:2517:C:C4	3.07	0.43
1:A:1187:G:H5''	17:2:76:LYS:HZ3	1.84	0.43
21:V:144:LEU:HB2	21:V:174:VAL:HG21	2.01	0.43
1:A:601:C:O2'	1:A:605:C:H5''	2.18	0.43
1:A:2694:G:H2'	1:A:2695:C:H6	1.84	0.43
18:S:110:LYS:HG3	18:S:111:HIS:CD2	2.53	0.43
28:6:11:LEU:HD23	28:6:51:GLU:CD	2.40	0.43
10:N:66:LYS:NZ	10:N:80:ASP:O	2.48	0.43
1:A:244:A:O3'	11:O:74:GLU:HB3	2.18	0.43
1:A:653:A:H5''	1:A:654:A:OP1	2.18	0.43
26:4:26:SER:OG	26:4:27:THR:N	2.51	0.43
1:A:890:A:H2'	1:A:892:G:C8	2.54	0.43
1:A:1068:G:C2	1:A:1069:A:C4	3.07	0.43
7:H:61:HIS:HA	7:H:64:LEU:HD12	2.00	0.43
1:A:2666:C:N4	7:H:152:ARG:HH22	2.17	0.43
21:V:150:LEU:HD22	21:V:154:ASP:CG	2.39	0.43
1:A:2314:C:O2'	1:A:2315:G:H5'	2.18	0.43
1:A:35:G:H2'	1:A:36:G:O4'	2.19	0.43
1:A:1534:G:H5'	1:A:1535:U:OP2	2.19	0.43
1:A:1359:A:H2'	1:A:1360:A:H5'	2.00	0.43
1:A:2378:A:O2'	14:Q:23:ARG:HD2	2.19	0.43
15:R:74:ARG:HD3	15:R:76:PHE:CZ	2.54	0.43
6:G:178:PHE:HA	6:G:179:PRO:HD2	1.66	0.43
30:8:50:LEU:O	30:8:51:ALA:HB2	2.18	0.43
1:A:1607:C:N4	1:A:1622:G:OP2	2.42	0.43
1:A:1255:U:C5	5:F:73:ALA:HA	2.54	0.43
1:A:2198:A:OP1	8:K:33:ARG:NH2	2.51	0.43
1:A:1363:C:O2'	1:A:1809:A:N3	2.44	0.43
23:Z:4:VAL:HG12	23:Z:11:ARG:HB3	2.01	0.43
1:A:899:A:O2'	1:A:900:A:H5'	2.19	0.43
8:K:122:GLU:HB3	8:K:126:TYR:OH	2.18	0.43
1:A:250:G:H5'	11:O:60:MET:HE1	2.01	0.42
1:A:2115:G:N2	1:A:2172:U:C4	2.87	0.42
1:A:2168:G:N1	1:A:2170:A:H8	2.15	0.42
20:U:54:LYS:C	20:U:55:TYR:CD2	2.92	0.42
1:A:1097:U:C4	1:A:1098:A:C5	3.07	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2665:A:H2'	1:A:2666:C:C6	2.54	0.42
1:A:1036:G:O6	1:A:1119:C:N4	2.39	0.42
2:B:104:A:O4'	21:V:29:TYR:HE2	2.02	0.42
21:V:68:PRO:O	21:V:91:LEU:N	2.52	0.42
16:1:72:HIS:CD2	16:1:110:VAL:HG21	2.46	0.42
23:Z:87:PRO:O	23:Z:88:LYS:C	2.58	0.42
8:K:76:THR:CG2	8:K:140:LEU:HD13	2.49	0.42
1:A:139:G:H22	1:A:1596:A:H4'	1.84	0.42
1:A:1576:U:H2'	1:A:1577:C:H6	1.84	0.42
4:E:144:ARG:HB3	4:E:145:LYS:H	1.37	0.42
30:8:23:VAL:HG22	30:8:47:LYS:HB3	2.01	0.42
4:E:169:ASN:HD22	4:E:169:ASN:C	2.23	0.42
1:A:2607:G:H2'	1:A:2608:G:O4'	2.18	0.42
1:A:528:A:H2	1:A:2043:C:C5'	2.31	0.42
15:R:10:VAL:O	15:R:12:SER:N	2.52	0.42
8:K:56:LYS:O	8:K:60:GLU:HB2	2.19	0.42
25:X:9:VAL:HG12	25:X:32:GLN:HE22	1.84	0.42
13:0:24:GLN:HB3	13:0:44:LEU:HD11	2.01	0.42
16:1:92:ARG:HH22	17:2:10:LYS:HB3	1.84	0.42
1:A:994:C:O2	17:2:10:LYS:HE2	2.19	0.42
1:A:2115:G:O2'	1:A:2165:G:N2	2.52	0.42
5:F:3:GLU:CA	5:F:24:LEU:HD11	2.41	0.42
17:2:71:LEU:HA	17:2:86:GLY:HA2	2.01	0.42
1:A:1614:A:N6	18:S:88:ARG:H	2.17	0.42
1:A:2294:C:P	14:Q:89:ARG:HH22	2.42	0.42
1:A:1545:A:N6	1:A:1545(A):A:N1	2.66	0.42
30:8:24:ALA:O	30:8:47:LYS:HA	2.19	0.42
24:W:13:ALA:HA	24:W:16:LEU:CD2	2.48	0.42
1:A:1252:G:O4'	16:1:33:ARG:HD2	2.20	0.42
16:1:68:ALA:O	16:1:71:GLN:HB3	2.18	0.42
5:F:152:GLU:HA	5:F:190:GLU:OE2	2.20	0.42
10:N:104:ARG:N	10:N:122:LEU:O	2.52	0.42
9:M:54:VAL:HB	9:M:122:VAL:HG22	2.01	0.42
4:E:9:VAL:HG23	4:E:10:GLY:N	2.34	0.42
1:A:2346:A:H5''	1:A:2383:G:H1'	2.01	0.42
4:E:53:PRO:HA	4:E:74:PRO:HA	2.02	0.42
1:A:2169:A:N1	1:A:2170:A:C4	2.87	0.42
1:A:1073:A:H2'	1:A:1074:G:C8	2.54	0.42
1:A:2747:G:OP1	7:H:138:LYS:HE2	2.18	0.42
7:H:7:LEU:N	7:H:8:PRO:HD2	2.34	0.42
3:D:147:LEU:HA	3:D:147:LEU:HD13	1.90	0.42
6:G:61:ALA:HB2	6:G:68:PRO:HD3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2:G:H22	1:A:2901:C:N4	2.16	0.42
1:A:1178:C:N4	1:A:1179:C:N3	2.67	0.42
20:U:68:HIS:H	20:U:71:LYS:NZ	2.18	0.42
1:A:2568:C:H2'	1:A:2569:G:O4'	2.19	0.42
1:A:2765:A:H2	1:A:2766:G:O4'	2.02	0.42
12:P:32:TYR:OH	12:P:133:ARG:NH2	2.52	0.42
1:A:128:C:H2'	1:A:129:C:H6	1.85	0.42
15:R:16:ARG:NH2	15:R:19:LEU:HD21	2.35	0.42
1:A:858:U:O2	1:A:2268:A:H2'	2.19	0.42
1:A:1246:A:OP1	5:F:38:ARG:NH1	2.51	0.42
11:O:87:ASP:O	11:O:90:ARG:HD3	2.19	0.42
1:A:724:U:H2'	1:A:725:G:O4'	2.19	0.42
1:A:2590:A:OP2	3:D:238:GLY:HA2	2.20	0.42
3:D:71:ASP:CG	3:D:103:ARG:HH22	2.22	0.42
4:E:73:GLU:HA	4:E:73:GLU:OE2	2.18	0.42
5:F:23:ASP:O	5:F:115:ALA:HA	2.18	0.42
6:G:105:LYS:CD	26:4:26:SER:HB3	2.49	0.42
2:B:89:G:C4	2:B:89(A):A:C2	3.08	0.42
1:A:1046:A:H5''	1:A:1047:G:C5'	2.49	0.42
1:A:1569:A:O5'	3:D:59:LYS:NZ	2.40	0.42
16:1:66:ASN:ND2	16:1:70:ARG:HE	2.14	0.42
14:Q:83:LYS:HZ2	14:Q:84:GLN:HG2	1.84	0.42
1:A:2401:U:O2	1:A:2402:C:C5	2.73	0.42
8:K:125:GLU:HA	8:K:141:LYS:HA	2.02	0.42
22:3:50:ASN:C	22:3:62:LEU:HD12	2.39	0.42
1:A:721:C:H2'	1:A:722:A:C8	2.54	0.42
1:A:515:A:H1'	1:A:581:C:H1'	2.02	0.42
1:A:70:G:OP1	1:A:112:U:N3	2.43	0.42
1:A:243:U:OP2	30:8:8:LYS:HE2	2.19	0.42
3:D:164:GLN:OE1	3:D:176:ARG:NH2	2.40	0.42
3:D:34:VAL:HG11	3:D:103:ARG:HA	2.01	0.42
1:A:390:A:C6	11:O:71:VAL:CG2	3.00	0.42
12:P:16:ARG:O	12:P:17:LEU:HD23	2.19	0.42
1:A:1538:G:H2'	1:A:1539:G:C8	2.54	0.42
17:2:32:THR:HA	17:2:60:GLU:HA	2.01	0.42
19:T:51:VAL:HA	19:T:83:VAL:HA	2.01	0.42
1:A:2698:U:H2'	1:A:2699:C:C6	2.54	0.42
16:1:85:LYS:HB2	16:1:116:ALA:HB1	2.01	0.42
1:A:2685:G:OP1	15:R:51:ARG:NH2	2.50	0.42
1:A:90:U:H2'	1:A:91:A:H5''	2.02	0.42
1:A:2563:U:O2	1:A:2565:A:C8	2.72	0.42
16:1:92:ARG:HD2	17:2:11:GLN:OE1	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:389:G:H8	1:A:389:G:O5'	2.03	0.42
28:6:15:GLU:HG3	28:6:47:THR:HG23	1.97	0.42
4:E:58:ARG:O	4:E:60:ASN:ND2	2.52	0.42
5:F:22:ALA:C	5:F:24:LEU:H	2.23	0.42
26:4:43:TYR:O	26:4:44:THR:C	2.58	0.42
6:G:109:VAL:HG13	26:4:33:VAL:HG23	2.01	0.42
7:H:67:LEU:HA	7:H:70:THR:HG22	2.01	0.42
1:A:2732:G:H3'	1:A:2733:A:O4'	2.18	0.42
1:A:1728:G:H8	1:A:1732:A:N6	2.10	0.42
2:B:15:A:O2'	2:B:109:G:C8	2.70	0.42
1:A:443:A:H5''	1:A:444:C:OP1	2.19	0.42
1:A:1299:G:H5'	1:A:1301:A:O4'	2.20	0.42
23:Z:88:LYS:HE2	23:Z:88:LYS:HB3	1.85	0.42
8:K:78:THR:OG1	8:K:104:GLN:OE1	2.37	0.42
1:A:752:A:H4'	1:A:753:C:O5'	2.19	0.42
25:X:39:ASP:OD1	25:X:44:ARG:NH2	2.39	0.42
1:A:835:A:OP1	30:8:52:LYS:HD3	2.20	0.42
1:A:566:U:H5''	11:O:29:LYS:HE3	2.02	0.42
1:A:492:A:H2'	1:A:493:G:O4'	2.20	0.42
1:A:2679:A:H4'	4:E:165:VAL:HG11	2.02	0.42
1:A:2361:A:O5'	30:8:27:THR:OG1	2.37	0.42
28:6:25:LYS:HB2	28:6:26:ASN:H	1.54	0.42
28:6:44:ARG:CG	28:6:45:LYS:H	2.32	0.42
1:A:2371:G:H5'	28:6:45:LYS:HE2	2.01	0.42
1:A:2133:G:N2	1:A:2157:G:H2'	2.35	0.42
1:A:882:G:C2	1:A:883:G:C8	3.07	0.42
1:A:2849:U:OP2	15:R:95:ARG:NH1	2.53	0.42
18:S:66:GLU:O	18:S:68:ARG:N	2.42	0.42
1:A:2299:G:N1	1:A:2318:G:C8	2.88	0.42
1:A:1113:U:H2'	1:A:1114:G:H8	1.84	0.42
13:O:34:ILE:HD12	13:O:34:ILE:HA	1.90	0.42
1:A:140:A:H8	1:A:1408:C:O2'	2.02	0.42
23:Z:81:LYS:H	23:Z:82:LEU:HD23	1.83	0.42
1:A:185:U:H2'	1:A:186:G:C8	2.55	0.42
1:A:997:G:OP1	16:1:93:LYS:HD3	2.20	0.42
16:1:97:ASP:OD2	16:1:101:ARG:NE	2.53	0.42
6:G:108:ASN:OD1	6:G:108:ASN:N	2.50	0.42
1:A:1066:U:H1'	1:A:1073:A:N1	2.35	0.42
1:A:1096:A:C6	1:A:1097:U:C2	3.08	0.42
2:B:30:C:N4	2:B:54:G:H1	2.07	0.42
1:A:1332:G:H5'	1:A:1332:G:C8	2.55	0.42
1:A:2665:A:H2'	1:A:2666:C:H6	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2139:C:N4	1:A:2152:G:H1	2.12	0.42
1:A:2652:C:N4	1:A:2668:G:H1	2.09	0.42
1:A:2210:G:H5'	1:A:2211:G:C6	2.55	0.42
1:A:2212:A:H4'	1:A:2213:U:N3	2.35	0.42
1:A:1394:U:H4'	1:A:1603:A:H4'	2.02	0.42
11:O:144:GLU:HA	11:O:145:PRO:HD3	1.81	0.42
10:N:1:MET:HB2	10:N:32:TYR:HB3	2.02	0.42
4:E:16:ARG:NH2	4:E:171:GLU:OE1	2.49	0.42
15:R:88:ILE:HD11	15:R:91:ARG:HG2	2.01	0.42
1:A:270(N):G:O2'	1:A:270(O):U:H5'	2.19	0.42
1:A:1461:G:H2'	1:A:1462:C:H6	1.85	0.42
1:A:1726:G:C6	1:A:1727:U:C4	3.08	0.42
6:G:125:PHE:HB3	6:G:166:ASP:HB2	2.02	0.42
1:A:957:A:N6	1:A:2459:A:C8	2.88	0.42
1:A:588:U:H1'	5:F:90:PHE:HB3	2.02	0.42
16:1:29:SER:C	16:1:30:LYS:HD2	2.40	0.42
10:N:79:PHE:CD2	15:R:72:VAL:HG22	2.54	0.42
24:W:25:VAL:O	24:W:29:LYS:HG3	2.19	0.42
18:S:13:SER:HA	18:S:99:ARG:HB2	2.02	0.42
23:Z:23:LYS:HD2	23:Z:28:GLY:HA3	2.01	0.42
27:5:36:CYS:HB3	27:5:37:LYS:H	1.65	0.42
1:A:755:C:H2'	1:A:756:C:C6	2.55	0.42
18:S:23:LEU:HD12	18:S:23:LEU:HA	1.87	0.42
15:R:50:ILE:HD13	15:R:50:ILE:HA	1.76	0.42
1:A:2286:A:H5'	28:6:28:ARG:NE	2.34	0.42
1:A:2116:G:N1	1:A:2165:G:O6	2.52	0.42
20:U:52:SER:N	20:U:53:PRO:HD3	2.35	0.42
2:B:87:G:O2'	2:B:89:G:O6	2.32	0.42
7:H:107:VAL:HB	7:H:109:PHE:HE1	1.84	0.42
1:A:1012:U:O4	9:M:28:THR:HG21	2.19	0.42
16:1:66:ASN:CG	16:1:76:TYR:HB2	2.40	0.42
21:V:100:VAL:O	21:V:124:ILE:HG22	2.19	0.42
1:A:1465:G:H4'	1:A:1528:A:H1'	2.01	0.42
15:R:61:PHE:CE1	15:R:76:PHE:HB2	2.55	0.42
1:A:1460:A:H4'	1:A:1461:G:OP2	2.20	0.42
1:A:1914:C:H2'	1:A:1915:U:O4'	2.19	0.42
16:1:100:VAL:O	16:1:102:GLU:N	2.40	0.42
1:A:1257:C:H4'	5:F:83:PHE:CE1	2.54	0.42
12:P:72:LYS:HA	12:P:73:PRO:HD3	1.75	0.42
7:H:122:THR:C	7:H:123:PHE:CG	2.93	0.42
1:A:1788:C:H2'	1:A:1789:A:O4'	2.19	0.42
1:A:246:C:OP1	11:O:70:GLN:O	2.38	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:185:U:H4'	1:A:218:A:H4'	2.02	0.42
1:A:1508:A:H4'	1:A:1510:A:C2	2.55	0.42
1:A:2848:G:C8	15:R:97:ALA:HB2	2.55	0.42
18:S:47:VAL:HA	18:S:50:VAL:HG12	2.01	0.42
1:A:1280:G:OP1	13:O:33:ARG:NH1	2.53	0.42
8:K:95:LYS:O	8:K:99:GLU:HG3	2.20	0.42
4:E:23:VAL:HG11	4:E:183:LEU:HB3	2.01	0.42
1:A:2124:G:H3'	1:A:2125:G:C8	2.55	0.42
1:A:1063:G:N2	1:A:1064:C:HO2'	2.18	0.42
1:A:2628:C:H1'	1:A:2781:A:H2'	2.02	0.42
1:A:2795:G:H1'	1:A:2802:G:H1	1.85	0.42
26:4:60:GLN:N	26:4:60:GLN:OE1	2.49	0.42
1:A:1115:G:H2'	1:A:1116:C:C6	2.54	0.42
12:P:23:GLY:CA	12:P:25:ASP:HB2	2.50	0.42
14:Q:62:LYS:HB3	14:Q:97:ARG:HD3	2.02	0.42
20:U:20:TYR:CZ	20:U:42:VAL:HA	2.55	0.42
1:A:903:C:H2'	1:A:904:C:C6	2.55	0.42
15:R:1:MET:HB3	15:R:2:ASN:H	1.43	0.42
1:A:1191:G:OP1	11:O:18:ARG:NH1	2.37	0.42
1:A:2843:G:H1	1:A:2874:C:N4	2.18	0.42
27:5:48:GLU:HA	27:5:56:LYS:NZ	2.35	0.42
11:O:110:TYR:HB3	11:O:111:ARG:H	1.59	0.42
7:H:10:PRO:HD2	7:H:50:VAL:O	2.20	0.42
1:A:1788:C:H5''	3:D:225:ALA:CB	2.50	0.42
19:T:67:GLY:O	19:T:69:TYR:N	2.46	0.42
14:Q:59:LYS:HD3	14:Q:60:GLY:H	1.85	0.42
1:A:1288:U:C2	1:A:1327:C:O2	2.73	0.42
28:6:30:THR:HA	28:6:31:PRO:HA	1.74	0.42
11:O:62:LEU:HD13	11:O:62:LEU:HA	1.79	0.41
1:A:1096:A:OP2	1:A:1096:A:H8	2.03	0.41
2:B:116:G:H2'	2:B:117:G:O4'	2.20	0.41
1:A:2342:C:O2	1:A:2374:C:H4'	2.20	0.41
1:A:2794:C:C4	1:A:2795:G:C5	3.07	0.41
2:B:52:A:N6	14:Q:33:LYS:HG2	2.35	0.41
1:A:2876:G:O5'	15:R:3:ARG:HA	2.20	0.41
1:A:1591:G:H2'	1:A:1592:C:C6	2.54	0.41
1:A:1465:G:N3	1:A:1545(A):A:H2	2.17	0.41
1:A:2191:G:O2'	1:A:2192:G:P	2.78	0.41
1:A:960:A:H5''	1:A:961:C:OP1	2.19	0.41
1:A:1935:G:O2'	1:A:1936:A:H5''	2.20	0.41
21:V:108:PRO:HB3	21:V:144:LEU:HD21	2.01	0.41
1:A:469:G:C6	29:7:39:ARG:NH1	2.88	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
16:1:39:LEU:HD23	16:1:39:LEU:HA	1.79	0.41
12:P:2:LEU:HD13	12:P:69:PHE:CD1	2.55	0.41
3:D:168:ARG:HG2	3:D:173:VAL:HG12	2.02	0.41
1:A:118:A:OP2	1:A:119:A:H2'	2.20	0.41
1:A:2678:C:H2'	1:A:2679:A:O4'	2.20	0.41
12:P:77:LYS:O	12:P:79:LEU:N	2.53	0.41
3:D:244:ARG:HB2	3:D:245:PRO:HD2	2.01	0.41
3:D:61:LEU:HA	3:D:61:LEU:HD12	1.79	0.41
4:E:9:VAL:CG1	4:E:26:ILE:O	2.68	0.41
26:4:36:CYS:HB3	26:4:39:CYS:HB2	1.32	0.41
1:A:2470:G:H5'	12:P:56:ARG:NH2	2.35	0.41
3:D:246:PRO:O	3:D:254:THR:HG22	2.21	0.41
6:G:119:GLY:O	6:G:181:ARG:HG3	2.20	0.41
1:A:1266:G:O2'	1:A:2012:G:O6	2.24	0.41
29:7:32:LYS:HZ3	29:7:32:LYS:HB3	1.84	0.41
30:8:60:LEU:O	30:8:61:LEU:HD12	2.19	0.41
1:A:1461:G:H2'	1:A:1462:C:C6	2.55	0.41
22:3:46:LYS:HA	22:3:47:PRO:HD3	1.81	0.41
4:E:143:ASN:HD22	4:E:147:PRO:HD3	1.85	0.41
1:A:1342:A:C2	1:A:1602:U:N3	2.86	0.41
17:2:89:GLN:HA	17:2:90:PRO:HD3	1.83	0.41
12:P:68:ILE:HD13	12:P:103:MET:HG2	2.02	0.41
5:F:29:ASN:HA	5:F:30:PRO:HD2	1.76	0.41
8:K:101:LEU:HA	8:K:105:HIS:HB2	2.01	0.41
1:A:944:G:H5''	1:A:945:A:O5'	2.19	0.41
1:A:2393:A:P	30:8:30:ARG:HB3	2.60	0.41
4:E:76:ARG:HG2	4:E:195:LEU:HD13	2.02	0.41
1:A:2134:A:N7	1:A:2158:A:C8	2.88	0.41
1:A:2638:G:O2'	1:A:2639:A:H8	2.02	0.41
1:A:1056:G:O2'	1:A:1086:A:O2'	2.19	0.41
1:A:2747:G:O2'	1:A:2748:A:O4'	2.38	0.41
7:H:4:ILE:HB	7:H:5:GLY:H	1.72	0.41
7:H:109:PHE:HZ	7:H:152:ARG:HB2	1.84	0.41
1:A:1479:G:O2'	1:A:1558:A:H5'	2.21	0.41
19:T:53:LYS:NZ	19:T:55:ASN:OD1	2.49	0.41
11:O:98:GLU:HA	11:O:101:VAL:HB	2.02	0.41
5:F:170:LEU:HA	5:F:170:LEU:HD23	1.90	0.41
9:M:16:ILE:HB	9:M:54:VAL:HG22	2.01	0.41
1:A:1161:C:O2'	17:2:8:GLY:HA2	2.20	0.41
1:A:194:G:H2'	1:A:195:A:O4'	2.20	0.41
1:A:448:U:H1'	5:F:84:VAL:HG13	2.02	0.41
1:A:821:A:H2'	1:A:946:G:H5''	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
17:2:37:VAL:O	17:2:51:VAL:HG13	2.18	0.41
17:2:52:VAL:HG13	17:2:55:ALA:HB3	2.01	0.41
1:A:2154:G:C4	1:A:2155:G:C8	3.08	0.41
4:E:37:ARG:HB2	4:E:46:ALA:O	2.21	0.41
1:A:896:A:OP2	21:V:146:ILE:HD11	2.20	0.41
1:A:1065:U:C2	1:A:1074:G:C2	3.08	0.41
1:A:2328:A:H2'	1:A:2329:G:C8	2.55	0.41
24:W:27:GLU:O	24:W:31:GLU:HG3	2.20	0.41
11:O:122:PRO:HA	11:O:142:GLY:N	2.34	0.41
1:A:273(D):C:N4	1:A:273(E):U:O4	2.53	0.41
1:A:2526:G:H5'	1:A:2742:C:O2'	2.21	0.41
1:A:1475:G:C2	1:A:1519:G:C2	3.08	0.41
1:A:685:A:C2	1:A:689:A:C6	3.08	0.41
13:O:38:VAL:HG22	13:O:112:ALA:HB2	2.02	0.41
23:Z:8:SER:HB3	23:Z:66:HIS:CD2	2.55	0.41
1:A:2420:C:OP2	30:8:34:TRP:CD2	2.73	0.41
11:O:3:LEU:HD12	11:O:3:LEU:H	1.86	0.41
1:A:1313:U:H2'	1:A:1610:A:N1	2.36	0.41
1:A:2141:G:C6	1:A:2151:G:C6	3.09	0.41
1:A:2472:G:H1'	1:A:2478:A:H61	1.86	0.41
15:R:64:ARG:CB	15:R:73:GLU:HG2	2.48	0.41
1:A:2211:G:O2'	1:A:2212:A:OP1	2.28	0.41
1:A:1525:G:H2'	1:A:1526:G:C8	2.55	0.41
3:D:70:TRP:HH2	3:D:152:GLY:H	1.69	0.41
19:T:49:VAL:HG23	19:T:51:VAL:HG23	2.02	0.41
2:B:39:A:N6	26:4:1:MET:HB2	2.35	0.41
8:K:98:ALA:HA	8:K:109:ILE:HD11	2.01	0.41
22:3:29:GLN:O	22:3:67:VAL:HG23	2.20	0.41
9:M:89:LYS:O	9:M:93:THR:OG1	2.39	0.41
1:A:2887:U:H2'	1:A:2888:C:C6	2.53	0.41
1:A:2086:U:H2'	1:A:2087:G:H8	1.84	0.41
6:G:63:ILE:HG22	6:G:143:GLU:HB2	2.01	0.41
5:F:155:LEU:HD12	5:F:155:LEU:HA	1.91	0.41
1:A:1878:G:H2'	1:A:1879:C:C6	2.55	0.41
24:W:47:ASN:O	24:W:49:LYS:N	2.54	0.41
1:A:2330:G:H4'	22:3:44:ARG:HH12	1.85	0.41
1:A:1356:G:H2'	1:A:1357:U:O4'	2.21	0.41
17:2:25:LEU:HA	17:2:25:LEU:HD23	1.85	0.41
16:1:114:LYS:H	16:1:114:LYS:HG2	1.50	0.41
4:E:26:ILE:CG2	4:E:27:LEU:N	2.66	0.41
28:6:18:ARG:O	28:6:19:ARG:HB3	2.21	0.41
4:E:76:ARG:C	4:E:78:LEU:H	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2135:A:H3'	1:A:2136:C:C6	2.56	0.41
1:A:2156:G:C6	1:A:2157:G:C2	3.08	0.41
26:4:16:CYS:HA	26:4:33:VAL:HG13	2.03	0.41
1:A:82:G:N1	1:A:103:A:OP2	2.53	0.41
1:A:2889:C:H3'	1:A:2891:G:C8	2.51	0.41
1:A:1188:U:O2'	1:A:1189:A:H5'	2.20	0.41
1:A:811:U:O2'	11:O:21:ARG:HG3	2.20	0.41
1:A:2823:A:OP1	4:E:159:HIS:NE2	2.51	0.41
6:G:173:LEU:HB3	6:G:178:PHE:CD2	2.55	0.41
1:A:315:G:C6	1:A:316:C:C4	3.09	0.41
10:N:47:ILE:HD12	10:N:47:ILE:HA	1.83	0.41
1:A:581:C:OP1	16:1:33:ARG:HG3	2.20	0.41
1:A:583:G:OP2	16:1:10:ARG:HD2	2.20	0.41
30:8:49:VAL:HG13	30:8:50:LEU:N	2.35	0.41
1:A:1254:A:H5''	1:A:1255:U:H5'	2.02	0.41
13:0:18:LEU:HD22	13:0:22:ARG:CD	2.50	0.41
1:A:1659:U:C4	1:A:1660:C:C5	3.09	0.41
11:O:49:ARG:NE	30:8:59:LYS:HD3	2.36	0.41
1:A:2134:A:H2	1:A:2159:G:H1'	1.86	0.41
1:A:2155:G:C5	1:A:2156:G:C5	3.08	0.41
1:A:2157:G:H2'	1:A:2158:A:C8	2.55	0.41
6:G:104:GLU:OE2	6:G:108:ASN:ND2	2.54	0.41
1:A:61:G:H1	1:A:93:C:H42	1.66	0.41
8:K:144:VAL:HG13	8:K:145:VAL:O	2.21	0.41
7:H:82:GLY:O	7:H:135:GLY:N	2.48	0.41
14:Q:65:VAL:O	14:Q:68:GLN:HB2	2.21	0.41
7:H:46:GLU:CD	7:H:51:ARG:HD2	2.41	0.41
1:A:1338:G:N7	19:T:62:LYS:NZ	2.63	0.41
1:A:319:C:H2'	1:A:320:A:O4'	2.21	0.41
7:H:122:THR:HB	7:H:124:GLU:OE2	2.21	0.41
1:A:196:A:O2'	1:A:805:G:O6	2.20	0.41
16:1:105:VAL:O	16:1:109:LEU:HG	2.21	0.41
1:A:2773:C:H2'	1:A:2774:C:H6	1.85	0.41
1:A:1000:A:C6	1:A:1001:A:N1	2.88	0.41
23:Z:5:CYS:HG	23:Z:8:SER:HG	1.66	0.41
30:8:16:ILE:HD13	30:8:57:ARG:HG3	2.01	0.41
1:A:1626:G:H5''	1:A:1627:G:H5'	2.03	0.41
1:A:2312:U:O5'	6:G:74:LYS:NZ	2.54	0.41
1:A:2128:C:C4	1:A:2129:C:C4	3.08	0.41
1:A:2637:U:H2'	1:A:2638:G:O4'	2.21	0.41
1:A:1053:C:N4	1:A:1054:A:C6	2.88	0.41
1:A:2341:G:H2'	1:A:2342:C:C6	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1045:A:H4'	1:A:1047:G:C5'	2.51	0.41
1:A:83:G:C2	1:A:102:G:H2'	2.56	0.41
10:N:106:LEU:HD23	10:N:106:LEU:HA	1.83	0.41
21:V:139:VAL:HG12	21:V:140:ASP:H	1.85	0.41
14:Q:34:HIS:ND1	14:Q:53:SER:HB2	2.36	0.41
3:D:133:LEU:HB2	3:D:187:GLY:HA2	2.02	0.41
1:A:1287:A:C5	1:A:1288:U:C4	3.08	0.41
24:W:30:ARG:NH2	24:W:34:GLU:OE2	2.32	0.41
1:A:49:A:H4'	1:A:50:U:O5'	2.20	0.41
1:A:49:A:H5'	1:A:51:G:O4'	2.20	0.41
1:A:1814:G:C6	1:A:1815:A:C6	3.08	0.41
1:A:2580:U:C5	1:A:2581:G:C6	3.08	0.41
12:P:38:GLU:OE1	12:P:128:LYS:N	2.47	0.41
16:1:27:LEU:HD22	16:1:31:SER:HB2	2.03	0.41
21:V:163:LEU:HD23	21:V:163:LEU:H	1.86	0.41
16:1:91:ASP:OD2	16:1:96:ALA:HB2	2.21	0.41
28:6:44:ARG:CZ	28:6:47:THR:HB	2.50	0.41
4:E:31:CYS:SG	4:E:51:PHE:HB2	2.60	0.41
1:A:1053:C:N3	1:A:1106:G:C2	2.89	0.41
1:A:1056:G:H5'	1:A:1086:A:N3	2.36	0.41
1:A:654(B):C:C2	1:A:654(T):A:C2	3.08	0.41
1:A:1044:G:H4'	1:A:1048:A:H1'	2.03	0.41
1:A:1047:G:C5	1:A:1110:G:O6	2.73	0.41
1:A:2798:C:H5''	1:A:2801:A:N6	2.36	0.41
1:A:885:C:H3'	1:A:886:C:C6	2.55	0.41
1:A:1678:G:N2	1:A:1989:G:N2	2.58	0.41
26:4:56:VAL:HG13	26:4:57:GLU:HG3	2.03	0.41
2:B:15:A:H3'	2:B:16:G:H5'	2.02	0.41
5:F:134:GLY:HA2	5:F:166:ALA:HB2	2.02	0.41
9:M:28:THR:O	9:M:32:THR:OG1	2.38	0.41
1:A:1178:C:C4	1:A:1179:C:C4	3.09	0.41
16:1:78:THR:OG1	16:1:79:PHE:N	2.53	0.41
1:A:1424:G:OP1	3:D:33:LEU:HD23	2.21	0.41
5:F:179:GLU:HA	5:F:205:ARG:HH22	1.86	0.41
1:A:1447:G:H1'	1:A:1545(A):A:H1'	2.02	0.41
19:T:27:THR:HG22	19:T:80:ILE:HG22	2.02	0.41
1:A:141:A:H1'	1:A:1408:C:O4'	2.21	0.41
1:A:276:A:H8	1:A:278:A:N7	2.19	0.41
1:A:275:G:H21	1:A:276:A:N6	2.19	0.41
27:5:56:LYS:HB3	27:5:57:VAL:H	1.58	0.41
1:A:171:G:H2'	1:A:172:C:C6	2.55	0.41
24:W:16:LEU:HD12	24:W:20:GLU:OE2	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:G:22:ARG:H	6:G:22:ARG:HG2	1.41	0.41
1:A:459:U:H2'	1:A:460:A:C8	2.55	0.41
21:V:23:LYS:HB3	21:V:38:TYR:CD1	2.56	0.41
1:A:118:A:OP2	1:A:119:A:H5''	2.20	0.41
5:F:130:ALA:H	5:F:142:TRP:HD1	1.67	0.41
1:A:1910:G:O2'	1:A:1911:U:H5'	2.21	0.41
9:M:96:GLU:HB2	9:M:122:VAL:HG12	2.02	0.41
20:U:35:TYR:CE2	20:U:69:ALA:HB3	2.56	0.41
1:A:2261:C:H1'	1:A:2388:A:N3	2.36	0.41
11:O:97:PRO:HD3	11:O:126:VAL:O	2.21	0.41
1:A:2018:G:H2'	1:A:2019:A:O4'	2.20	0.41
10:N:119:PRO:HB2	15:R:68:TYR:CE2	2.56	0.41
22:3:73:GLY:O	22:3:76:GLY:N	2.44	0.41
18:S:2:GLU:OE1	18:S:72:LYS:NZ	2.41	0.41
12:P:60:ARG:HA	12:P:60:ARG:HD3	1.86	0.41
7:H:118:PRO:HB2	7:H:119:GLU:H	1.53	0.41
4:E:38:THR:HA	4:E:39:PRO:HD2	1.82	0.41
9:M:68:GLU:HG2	9:M:88:GLU:OE1	2.21	0.41
16:1:108:GLU:OE1	17:2:45:THR:HA	2.21	0.41
1:A:2114:A:H61	1:A:2170:A:N6	2.18	0.41
1:A:1079:C:H41	1:A:1088:A:H5''	1.86	0.41
1:A:1093:G:H1'	1:A:1099:G:N1	2.36	0.41
1:A:1651:G:P	13:0:37:THR:HG21	2.61	0.41
1:A:2808:U:H2'	1:A:2809:A:H8	1.86	0.41
1:A:1039:G:C6	1:A:1040:C:C4	3.08	0.41
11:O:88:LEU:HD11	11:O:95:VAL:HG21	2.03	0.41
1:A:540:G:H1	1:A:553:U:H3	1.67	0.41
6:G:173:LEU:HD12	6:G:178:PHE:CZ	2.55	0.41
1:A:1761:C:H3'	1:A:1762:A:H5''	2.02	0.41
1:A:721:C:H2'	1:A:722:A:H8	1.86	0.41
1:A:975:G:H1'	1:A:990:A:C2	2.56	0.41
1:A:920:G:H2'	1:A:921:G:C8	2.54	0.41
8:K:128:LEU:O	8:K:138:ILE:HG22	2.21	0.41
21:V:43:GLU:O	21:V:47:VAL:HG23	2.21	0.41
26:4:10:VAL:HA	26:4:11:PRO:HD2	1.84	0.41
3:D:66:ASP:CG	3:D:68:LYS:O	2.59	0.41
1:A:18:C:O3'	16:1:23:GLY:HA2	2.21	0.41
16:1:99:ALA:HB2	16:1:106:PHE:CD1	2.56	0.41
19:T:40:LYS:O	19:T:42:ALA:N	2.45	0.41
1:A:2320:A:N6	1:A:2333:A:H2'	2.36	0.41
10:N:105:GLU:N	10:N:105:GLU:OE1	2.54	0.41
1:A:897:C:H5'	1:A:898:C:P	2.60	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1651:G:H2'	1:A:1652:A:O4'	2.21	0.40
16:1:41:ALA:HB1	16:1:45:TYR:CE2	2.56	0.40
2:B:44:G:P	6:G:98:ARG:HH22	2.43	0.40
17:2:60:GLU:HG2	17:2:97:LYS:HD3	2.04	0.40
21:V:52:SER:C	21:V:54:HIS:H	2.23	0.40
4:E:101:ARG:HA	4:E:170:LEU:O	2.21	0.40
14:Q:64:GLU:O	14:Q:68:GLN:HG2	2.20	0.40
1:A:1460:A:O2'	1:A:1461:G:OP2	2.33	0.40
22:3:53:MET:HG2	22:3:57:PHE:HA	2.02	0.40
1:A:870:A:OP1	12:P:6:ARG:NH1	2.48	0.40
1:A:820:A:C2	1:A:943:U:H4'	2.56	0.40
7:H:94:TYR:HA	7:H:106:THR:O	2.21	0.40
1:A:1342:A:H2	1:A:1602:U:N3	2.18	0.40
7:H:24:VAL:HB	7:H:25:LYS:H	1.52	0.40
5:F:155:LEU:N	5:F:191:ARG:O	2.42	0.40
15:R:85:LYS:NZ	15:R:87:ASP:OD2	2.47	0.40
1:A:1666:G:H1'	10:N:3:GLN:HE21	1.86	0.40
1:A:2344:U:OP1	28:6:38:LYS:HD2	2.21	0.40
5:F:7:TYR:CE2	5:F:16:GLY:HA3	2.55	0.40
5:F:4:VAL:HA	5:F:19:GLU:HB3	2.04	0.40
1:A:2095:C:H2'	1:A:2096:U:O4'	2.21	0.40
1:A:676:A:H1'	1:A:2443:C:O4'	2.21	0.40
1:A:2776:A:H4'	1:A:2777:G:O5'	2.21	0.40
1:A:1141:U:H2'	9:M:63:THR:HG21	2.02	0.40
1:A:2850:A:N7	1:A:2868:A:O2'	2.37	0.40
4:E:18:ASP:OD1	4:E:18:ASP:N	2.55	0.40
1:A:2401:U:O5'	1:A:2401:U:C6	2.74	0.40
20:U:46:LYS:O	20:U:47:LYS:C	2.59	0.40
1:A:1459:G:C2'	1:A:1460:A:H5'	2.51	0.40
1:A:2867:G:OP2	15:R:119:LYS:NZ	2.34	0.40
21:V:116:VAL:HG23	21:V:179:ASP:OD1	2.21	0.40
1:A:918:A:H5''	2:B:97:G:O2'	2.21	0.40
1:A:2557:G:H2'	1:A:2558:C:C6	2.57	0.40
1:A:858:U:H1'	1:A:2268:A:H2'	2.02	0.40
14:Q:59:LYS:HD3	14:Q:60:GLY:N	2.37	0.40
12:P:77:LYS:HA	12:P:78:PRO:HD3	1.93	0.40
7:H:15:VAL:HG23	7:H:17:VAL:HG23	2.03	0.40
19:T:32:PRO:HA	19:T:77:LYS:HB2	2.03	0.40
5:F:32:LEU:HB3	5:F:112:MET:HE1	2.03	0.40
1:A:1471:A:OP2	1:A:1521:G:N1	2.47	0.40
9:M:127:ASP:N	9:M:127:ASP:OD1	2.55	0.40
28:6:39:TYR:CD2	28:6:40:CYS:O	2.71	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2129:C:C4	1:A:2130:U:N3	2.90	0.40
1:A:2159:G:H2'	1:A:2160:G:O4'	2.21	0.40
5:F:3:GLU:HG3	5:F:19:GLU:HB2	2.02	0.40
1:A:1093:G:N2	1:A:1097:U:H5''	2.28	0.40
1:A:834:C:H1'	1:A:2358:G:N3	2.36	0.40
7:H:2:SER:OG	7:H:2:SER:O	2.39	0.40
1:A:1516:U:H2'	1:A:1517:G:H8	1.86	0.40
2:B:52:A:O3'	2:B:53:A:H8	2.05	0.40
1:A:872:A:H2'	1:A:873:G:C8	2.56	0.40
3:D:70:TRP:CZ3	3:D:146:GLU:OE2	2.74	0.40
1:A:1999:C:H5''	1:A:2723:C:O2'	2.21	0.40
5:F:164:ARG:HH12	5:F:177:ALA:HB2	1.87	0.40
1:A:2103:C:H2'	1:A:2104:G:C8	2.56	0.40
21:V:14:LYS:HA	21:V:15:PRO:HD2	1.89	0.40
1:A:134:C:N4	1:A:145:G:H1	2.20	0.40
4:E:2:LYS:HD2	4:E:95:ILE:CG2	2.51	0.40
1:A:51:G:N2	1:A:120:U:O2	2.50	0.40
1:A:1654:A:OP1	13:O:2:ARG:HD3	2.21	0.40
21:V:170:THR:O	21:V:172:ALA:N	2.54	0.40
16:1:92:ARG:HD3	16:1:95:LEU:HD12	2.04	0.40
1:A:2371:G:H4'	28:6:45:LYS:HD2	2.04	0.40
1:A:2125:G:O5'	1:A:2125:G:H8	2.04	0.40
1:A:892:G:H2'	1:A:893:C:C6	2.57	0.40
1:A:1088:A:O2'	1:A:1089:G:OP2	2.39	0.40
1:A:2745:C:H2'	1:A:2746:U:O4'	2.22	0.40
1:A:2795:G:N3	1:A:2802:G:C6	2.90	0.40
11:O:3:LEU:C	11:O:5:ASP:H	2.25	0.40
21:V:77:ASP:N	21:V:82:ARG:O	2.51	0.40
1:A:1516:U:H2'	1:A:1517:G:C8	2.57	0.40
1:A:1041:C:H2'	1:A:1042:G:C8	2.56	0.40
3:D:255:LYS:O	3:D:255:LYS:HD2	2.21	0.40
1:A:753:C:H6	1:A:753:C:O5'	2.03	0.40
22:3:25:ARG:HD2	22:3:29:GLN:HE22	1.85	0.40
24:W:10:LEU:O	24:W:14:ARG:N	2.27	0.40
11:O:98:GLU:HG2	11:O:99:LEU:N	2.36	0.40
1:A:363:G:H5'	1:A:363(A):A:OP2	2.22	0.40
1:A:185:U:H2'	1:A:186:G:H8	1.86	0.40
8:K:117:GLU:OE1	8:K:118:LYS:N	2.54	0.40
1:A:1850:G:H2'	1:A:1851:U:O4'	2.21	0.40
7:H:16:SER:HB2	7:H:27:LYS:HB3	2.03	0.40
1:A:946:G:H2'	1:A:947:G:C8	2.57	0.40
1:A:414:C:H4'	1:A:1879:C:O2	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:76:C:O3'	24:W:59:ARG:HG3	2.21	0.40
1:A:2712:U:HO2'	1:A:2712(A):A:P	2.45	0.40
22:3:36:ILE:HG13	22:3:58:THR:CG2	2.51	0.40
3:D:201:HIS:O	3:D:204:ILE:HG12	2.22	0.40
1:A:2101:G:C6	1:A:2102:U:C4	3.09	0.40
10:N:7:TYR:HE1	10:N:20:MET:HE3	1.86	0.40
6:G:4:ASP:HA	6:G:9:ARG:NH2	2.37	0.40
5:F:165:ARG:HH11	5:F:165:ARG:HB3	1.86	0.40
5:F:135:LYS:HA	5:F:135:LYS:HD2	1.82	0.40
4:E:52:LEU:HA	4:E:52:LEU:HD23	1.95	0.40
1:A:1072:C:C4	1:A:1093:G:C6	3.10	0.40
7:H:54:ARG:HB3	7:H:65:HIS:HB2	2.03	0.40
17:2:78:LYS:O	17:2:79:VAL:HG13	2.22	0.40
1:A:1174:A:C6	1:A:1176:G:H1'	2.56	0.40
14:Q:110:LEU:HD12	14:Q:111:GLU:H	1.86	0.40
14:Q:110:LEU:CD1	14:Q:111:GLU:H	2.34	0.40
10:N:1:MET:H1	10:N:67:LYS:HB3	1.86	0.40
10:N:67:LYS:HE3	10:N:68:GLU:OE1	2.21	0.40
1:A:270(L):U:O2'	1:A:270(N):G:N2	2.55	0.40
1:A:2736:G:H2'	1:A:2737:G:H8	1.85	0.40
1:A:688:U:H5'	1:A:1780:A:C2	2.56	0.40
1:A:1323:U:H2'	1:A:1324:G:H5'	2.03	0.40
1:A:558:G:P	9:M:111:PRO:HD2	2.62	0.40
20:U:63:LYS:HE3	20:U:64:GLU:OE2	2.21	0.40
1:A:2540:C:H2'	1:A:2541:A:O4'	2.22	0.40
1:A:1599:C:OP1	19:T:36:LYS:HG3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	270/276 (98%)	217 (80%)	40 (15%)	13 (5%)	4	23
4	E	203/206 (98%)	133 (66%)	33 (16%)	37 (18%)	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	F	206/210 (98%)	151 (73%)	29 (14%)	26 (13%)	0	3
6	G	179/182 (98%)	121 (68%)	38 (21%)	20 (11%)	1	5
7	H	168/180 (93%)	92 (55%)	45 (27%)	31 (18%)	0	0
8	K	144/148 (97%)	104 (72%)	28 (19%)	12 (8%)	1	9
9	M	136/140 (97%)	110 (81%)	22 (16%)	4 (3%)	7	38
10	N	120/122 (98%)	103 (86%)	14 (12%)	3 (2%)	9	42
11	O	148/150 (99%)	83 (56%)	44 (30%)	21 (14%)	0	2
12	P	139/141 (99%)	105 (76%)	19 (14%)	15 (11%)	1	5
13	0	115/118 (98%)	99 (86%)	13 (11%)	3 (3%)	8	41
14	Q	109/112 (97%)	78 (72%)	20 (18%)	11 (10%)	1	6
15	R	135/146 (92%)	110 (82%)	19 (14%)	6 (4%)	4	25
16	1	115/118 (98%)	88 (76%)	18 (16%)	9 (8%)	1	11
17	2	99/101 (98%)	73 (74%)	12 (12%)	14 (14%)	0	2
18	S	111/113 (98%)	98 (88%)	8 (7%)	5 (4%)	4	24
19	T	90/96 (94%)	69 (77%)	13 (14%)	8 (9%)	1	8
20	U	100/110 (91%)	53 (53%)	22 (22%)	25 (25%)	0	0
21	V	177/206 (86%)	111 (63%)	35 (20%)	31 (18%)	0	0
22	3	75/85 (88%)	66 (88%)	7 (9%)	2 (3%)	8	39
23	Z	95/98 (97%)	71 (75%)	14 (15%)	10 (10%)	1	5
24	W	67/72 (93%)	53 (79%)	6 (9%)	8 (12%)	1	4
25	X	57/60 (95%)	49 (86%)	5 (9%)	3 (5%)	3	21
26	4	61/71 (86%)	25 (41%)	18 (30%)	18 (30%)	0	0
27	5	57/60 (95%)	46 (81%)	7 (12%)	4 (7%)	2	13
28	6	43/54 (80%)	19 (44%)	13 (30%)	11 (26%)	0	0
29	7	47/49 (96%)	45 (96%)	2 (4%)	0	100	100
30	8	59/65 (91%)	42 (71%)	8 (14%)	9 (15%)	0	1
All	All	3325/3489 (95%)	2414 (73%)	552 (17%)	359 (11%)	1	5

All (359) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	26	LYS
3	D	32	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	267	SER
4	E	25	VAL
4	E	27	LEU
4	E	54	GLN
4	E	61	ARG
4	E	64	LYS
4	E	70	ALA
4	E	72	VAL
4	E	77	ILE
4	E	82	ARG
4	E	86	PRO
4	E	87	GLU
4	E	88	GLY
4	E	200	GLU
5	F	4	VAL
5	F	6	VAL
5	F	17	ARG
5	F	26	ALA
5	F	132	VAL
6	G	4	ASP
6	G	81	LYS
6	G	84	LYS
6	G	116	ASP
7	H	3	ARG
7	H	24	VAL
7	H	55	PRO
7	H	83	TYR
7	H	123	PHE
7	H	128	PRO
7	H	130	ARG
7	H	136	ILE
7	H	152	ARG
8	K	69	LYS
8	K	83	ALA
8	K	102	SER
8	K	117	GLU
8	K	132	PRO
11	O	10	PRO
11	O	21	ARG
11	O	46	LYS
11	O	49	ARG
11	O	50	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	O	56	SER
11	O	60	MET
11	O	61	ARG
11	O	62	LEU
11	O	63	PRO
12	P	7	MET
12	P	13	GLN
12	P	21	THR
12	P	66	ILE
12	P	89	ASN
14	Q	54	LEU
14	Q	88	ASP
14	Q	89	ARG
14	Q	96	GLY
14	Q	106	ARG
14	Q	110	LEU
15	R	2	ASN
15	R	134	GLU
16	1	91	ASP
17	2	47	VAL
17	2	50	PRO
17	2	79	VAL
20	U	44	ILE
20	U	50	ARG
20	U	53	PRO
20	U	56	PRO
20	U	77	PRO
20	U	78	ALA
20	U	85	VAL
20	U	89	PHE
21	V	53	ILE
21	V	60	GLU
21	V	93	ASP
21	V	112	ARG
21	V	114	GLY
21	V	120	ILE
21	V	131	ARG
21	V	135	GLU
21	V	146	ILE
21	V	159	PRO
21	V	176	PRO
23	Z	81	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
23	Z	83	GLU
23	Z	88	LYS
23	Z	93	GLU
24	W	17	SER
26	4	16	CYS
26	4	20	ASN
26	4	21	VAL
26	4	22	ILE
26	4	24	THR
26	4	33	VAL
26	4	40	HIS
26	4	44	THR
26	4	46	GLN
27	5	4	HIS
27	5	57	VAL
28	6	26	ASN
28	6	44	ARG
28	6	48	VAL
30	8	49	VAL
30	8	51	ALA
30	8	61	LEU
3	D	30	GLU
3	D	70	TRP
4	E	9	VAL
4	E	26	ILE
4	E	37	ARG
4	E	51	PHE
4	E	59	VAL
4	E	78	LEU
4	E	90	THR
5	F	10	PRO
5	F	27	GLU
5	F	28	ILE
5	F	61	GLY
5	F	67	GLN
5	F	70	THR
5	F	84	VAL
5	F	89	VAL
5	F	133	ASN
6	G	5	VAL
6	G	32	PRO
6	G	36	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	G	96	ARG
6	G	119	GLY
6	G	146	TYR
7	H	4	ILE
7	H	92	ILE
7	H	93	GLY
7	H	118	PRO
7	H	138	LYS
8	K	68	LEU
8	K	73	GLU
8	K	101	LEU
8	K	144	VAL
9	M	135	PRO
10	N	5	GLN
10	N	28	SER
11	O	6	LEU
11	O	57	THR
11	O	66	GLY
11	O	109	GLY
11	O	141	ALA
12	P	27	VAL
12	P	88	GLY
12	P	90	VAL
13	0	82	GLU
13	0	107	ASP
14	Q	57	LYS
14	Q	74	ALA
15	R	11	GLU
15	R	17	THR
16	1	72	HIS
16	1	90	VAL
16	1	93	LYS
16	1	98	LEU
16	1	100	VAL
17	2	48	GLY
17	2	49	THR
17	2	54	GLY
17	2	83	ARG
17	2	99	ILE
18	S	63	ASP
18	S	67	ASP
19	T	41	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	T	93	GLU
20	U	39	VAL
20	U	47	LYS
20	U	57	GLN
20	U	61	ILE
20	U	99	CYS
21	V	7	ALA
21	V	66	SER
21	V	90	VAL
21	V	105	VAL
21	V	140	ASP
21	V	142	SER
21	V	145	GLU
21	V	156	LYS
21	V	158	PRO
21	V	171	ILE
23	Z	27	GLU
23	Z	87	PRO
23	Z	92	LYS
24	W	48	HIS
24	W	70	GLN
25	X	38	GLU
26	4	26	SER
26	4	37	SER
26	4	43	TYR
27	5	49	CYS
28	6	17	LYS
28	6	45	LYS
30	8	30	ARG
30	8	32	LEU
30	8	41	ILE
3	D	3	VAL
3	D	110	GLY
4	E	24	THR
4	E	60	ASN
4	E	69	LYS
4	E	144	ARG
4	E	203	LYS
5	F	3	GLU
5	F	9	ILE
5	F	11	VAL
5	F	42	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	F	62	ARG
6	G	6	ALA
6	G	82	LEU
6	G	124	SER
6	G	179	PRO
7	H	17	VAL
7	H	21	PRO
7	H	27	LYS
7	H	90	LYS
7	H	98	LEU
7	H	99	VAL
7	H	112	PRO
7	H	127	GLU
7	H	150	ALA
7	H	164	TYR
9	M	3	THR
11	O	14	LYS
12	P	104	PHE
12	P	134	ARG
13	0	45	ARG
14	Q	19	LYS
14	Q	111	GLU
15	R	116	ALA
16	1	101	ARG
16	1	117	GLN
18	S	93	ALA
18	S	111	HIS
19	T	42	ALA
20	U	23	ARG
20	U	55	TYR
20	U	62	GLU
20	U	102	CYS
21	V	12	GLY
21	V	161	VAL
22	3	35	ASN
23	Z	28	GLY
24	W	10	LEU
24	W	47	ASN
25	X	13	ILE
26	4	10	VAL
26	4	27	THR
26	4	42	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	4	54	GLY
27	5	55	ARG
28	6	28	ARG
28	6	41	PRO
3	D	27	THR
3	D	156	ALA
3	D	268	ARG
4	E	22	PRO
4	E	57	LYS
4	E	68	ALA
5	F	14	PRO
5	F	123	LEU
5	F	167	ALA
6	G	62	LEU
6	G	104	GLU
7	H	85	LYS
7	H	167	GLU
8	K	26	ALA
8	K	30	LEU
9	M	47	ALA
10	N	26	LYS
11	O	35	HIS
11	O	55	ARG
12	P	25	ASP
12	P	78	PRO
14	Q	53	SER
15	R	126	ALA
16	1	94	ASN
17	2	85	LYS
19	T	23	GLU
19	T	40	LYS
20	U	29	GLU
20	U	52	SER
20	U	90	LEU
21	V	41	LEU
21	V	65	GLN
24	W	15	LYS
24	W	43	GLN
26	4	25	TYR
28	6	23	THR
30	8	48	PHE
30	8	53	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	239	ARG
4	E	52	LEU
4	E	73	GLU
4	E	76	ARG
6	G	21	ARG
6	G	138	GLN
6	G	150	ASP
7	H	65	HIS
7	H	117	PRO
7	H	137	ASP
7	H	155	SER
8	K	100	ALA
11	O	117	GLU
12	P	59	ARG
17	2	44	LYS
19	T	15	GLU
19	T	51	VAL
20	U	3	VAL
20	U	63	LYS
21	V	62	PRO
21	V	141	VAL
21	V	162	GLU
21	V	165	VAL
22	3	64	ASP
23	Z	30	VAL
26	4	57	GLU
28	6	19	ARG
28	6	25	LYS
28	6	36	LEU
30	8	7	HIS
4	E	7	VAL
4	E	65	GLY
5	F	113	ALA
6	G	147	ASP
12	P	79	LEU
17	2	38	LEU
17	2	84	LYS
18	S	65	LEU
19	T	67	GLY
20	U	80	GLY
21	V	148	ASP
24	W	16	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	24	ILE
4	E	50	GLY
4	E	75	VAL
4	E	116	VAL
4	E	186	GLY
5	F	24	LEU
5	F	114	VAL
25	X	27	GLY
5	F	16	GLY
21	V	157	LEU
3	D	271	ILE
12	P	47	ILE
20	U	42	VAL
20	U	98	VAL
23	Z	31	GLY
7	H	15	VAL
9	M	113	GLY
11	O	24	GLY
17	2	36	PRO
17	2	52	VAL
11	O	116	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	214/218 (98%)	183 (86%)	31 (14%)	5	18
4	E	165/166 (99%)	143 (87%)	22 (13%)	6	22
5	F	165/166 (99%)	138 (84%)	27 (16%)	3	12
6	G	155/156 (99%)	132 (85%)	23 (15%)	4	17
7	H	142/148 (96%)	109 (77%)	33 (23%)	1	5
8	K	122/124 (98%)	92 (75%)	30 (25%)	1	3
9	M	117/119 (98%)	96 (82%)	21 (18%)	2	10
10	N	100/100 (100%)	87 (87%)	13 (13%)	6	23
11	O	116/116 (100%)	84 (72%)	32 (28%)	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	P	111/111 (100%)	94 (85%)	17 (15%)	4	15
13	O	100/101 (99%)	89 (89%)	11 (11%)	9	34
14	Q	87/88 (99%)	69 (79%)	18 (21%)	2	8
15	R	120/127 (94%)	98 (82%)	22 (18%)	2	10
16	1	93/94 (99%)	79 (85%)	14 (15%)	4	16
17	2	82/82 (100%)	62 (76%)	20 (24%)	1	4
18	S	92/92 (100%)	75 (82%)	17 (18%)	2	9
19	T	74/78 (95%)	66 (89%)	8 (11%)	9	34
20	U	85/91 (93%)	59 (69%)	26 (31%)	0	1
21	V	158/179 (88%)	136 (86%)	22 (14%)	5	21
22	3	62/67 (92%)	58 (94%)	4 (6%)	24	65
23	Z	82/83 (99%)	76 (93%)	6 (7%)	20	59
24	W	64/67 (96%)	61 (95%)	3 (5%)	36	78
25	X	51/52 (98%)	43 (84%)	8 (16%)	4	14
26	4	57/63 (90%)	36 (63%)	21 (37%)	0	0
27	5	51/52 (98%)	43 (84%)	8 (16%)	4	14
28	6	44/52 (85%)	31 (70%)	13 (30%)	0	1
29	7	42/42 (100%)	33 (79%)	9 (21%)	1	7
30	8	51/55 (93%)	41 (80%)	10 (20%)	2	8
All	All	2802/2889 (97%)	2313 (82%)	489 (18%)	3	11

All (489) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	5	LYS
3	D	27	THR
3	D	31	LYS
3	D	35	LYS
3	D	44	ASN
3	D	46	GLN
3	D	61	LEU
3	D	64	ILE
3	D	65	ILE
3	D	87	ASN
3	D	94	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	99	ASP
3	D	103	ARG
3	D	105	ILE
3	D	106	ILE
3	D	109	ASP
3	D	116	GLN
3	D	118	VAL
3	D	141	VAL
3	D	147	LEU
3	D	150	LYS
3	D	157	ARG
3	D	192	THR
3	D	211	ARG
3	D	242	ARG
3	D	244	ARG
3	D	255	LYS
3	D	257	LEU
3	D	266	SER
3	D	270	ILE
3	D	271	ILE
4	E	33	VAL
4	E	35	GLN
4	E	40	GLU
4	E	54	GLN
4	E	69	LYS
4	E	76	ARG
4	E	78	LEU
4	E	79	ARG
4	E	91	VAL
4	E	108	SER
4	E	111	ARG
4	E	119	ARG
4	E	135	HIS
4	E	144	ARG
4	E	169	ASN
4	E	170	LEU
4	E	175	VAL
4	E	181	LEU
4	E	188	VAL
4	E	197	ILE
4	E	200	GLU
4	E	201	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	F	1	MET
5	F	2	LYS
5	F	3	GLU
5	F	4	VAL
5	F	7	TYR
5	F	8	GLN
5	F	11	VAL
5	F	19	GLU
5	F	20	LEU
5	F	23	ASP
5	F	33	LEU
5	F	63	LYS
5	F	67	GLN
5	F	68	LYS
5	F	74	ARG
5	F	100	THR
5	F	104	LYS
5	F	158	THR
5	F	181	LEU
5	F	183	VAL
5	F	192	LEU
5	F	195	ASP
5	F	196	LEU
5	F	197	ASP
5	F	200	GLU
5	F	201	VAL
5	F	205	ARG
6	G	3	LEU
6	G	5	VAL
6	G	20	ILE
6	G	22	ARG
6	G	26	GLN
6	G	43	LEU
6	G	47	LYS
6	G	48	GLU
6	G	53	LEU
6	G	67	LYS
6	G	88	ILE
6	G	90	LEU
6	G	91	ARG
6	G	92	VAL
6	G	94	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	G	100	TRP
6	G	108	ASN
6	G	116	ASP
6	G	133	LEU
6	G	139	LEU
6	G	145	THR
6	G	148	MET
6	G	165	THR
7	H	3	ARG
7	H	4	ILE
7	H	7	LEU
7	H	11	VAL
7	H	16	SER
7	H	24	VAL
7	H	30	LYS
7	H	32	GLU
7	H	41	MET
7	H	43	VAL
7	H	49	VAL
7	H	50	VAL
7	H	51	ARG
7	H	56	SER
7	H	67	LEU
7	H	71	LEU
7	H	74	ASN
7	H	83	TYR
7	H	88	LEU
7	H	89	ILE
7	H	101	ARG
7	H	103	LEU
7	H	104	GLU
7	H	105	LEU
7	H	121	ILE
7	H	123	PHE
7	H	129	THR
7	H	139	GLN
7	H	141	VAL
7	H	157	TYR
7	H	159	GLU
7	H	164	TYR
7	H	169	VAL
8	K	9	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	K	37	VAL
8	K	44	LEU
8	K	50	ARG
8	K	52	ARG
8	K	56	LYS
8	K	61	ARG
8	K	66	GLU
8	K	67	ARG
8	K	74	ASN
8	K	76	THR
8	K	77	LEU
8	K	78	THR
8	K	81	VAL
8	K	85	GLU
8	K	86	THR
8	K	87	LYS
8	K	104	GLN
8	K	109	ILE
8	K	113	ARG
8	K	117	GLU
8	K	118	LYS
8	K	125	GLU
8	K	131	LYS
8	K	133	HIS
8	K	135	GLU
8	K	136	VAL
8	K	142	VAL
8	K	144	VAL
8	K	145	VAL
9	M	7	LYS
9	M	9	VAL
9	M	15	LEU
9	M	22	THR
9	M	28	THR
9	M	29	LYS
9	M	32	THR
9	M	33	LEU
9	M	34	LEU
9	M	38	HIS
9	M	43	THR
9	M	48	MET
9	M	58	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	M	60	ILE
9	M	63	THR
9	M	65	LYS
9	M	69	GLN
9	M	87	LEU
9	M	93	THR
9	M	94	HIS
9	M	137	LYS
10	N	9	GLU
10	N	21	CYS
10	N	23	ARG
10	N	24	VAL
10	N	34	THR
10	N	47	ILE
10	N	49	ARG
10	N	70	LYS
10	N	78	ARG
10	N	80	ASP
10	N	87	ILE
10	N	89	ASN
10	N	94	ARG
11	O	6	LEU
11	O	21	ARG
11	O	30	THR
11	O	36	LYS
11	O	41	ARG
11	O	45	LEU
11	O	46	LYS
11	O	52	GLU
11	O	57	THR
11	O	58	THR
11	O	59	LEU
11	O	61	ARG
11	O	62	LEU
11	O	65	ARG
11	O	67	MET
11	O	81	GLN
11	O	83	VAL
11	O	85	LEU
11	O	91	PHE
11	O	95	VAL
11	O	96	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	O	98	GLU
11	O	105	LEU
11	O	110	TYR
11	O	111	ARG
11	O	114	ILE
11	O	125	VAL
11	O	138	LEU
11	O	139	LYS
11	O	144	GLU
11	O	147	LEU
11	O	148	LEU
12	P	1	MET
12	P	6	ARG
12	P	26	TYR
12	P	45	GLN
12	P	59	ARG
12	P	60	ARG
12	P	64	ILE
12	P	75	THR
12	P	83	MET
12	P	89	ASN
12	P	103	MET
12	P	110	THR
12	P	111	GLU
12	P	131	ILE
12	P	133	ARG
12	P	135	ASP
12	P	138	ASP
13	0	18	LEU
13	0	28	LEU
13	0	33	ARG
13	0	44	LEU
13	0	57	ARG
13	0	75	LEU
13	0	79	LEU
13	0	81	ASP
13	0	96	ARG
13	0	105	ARG
13	0	117	VAL
14	Q	5	THR
14	Q	12	PHE
14	Q	14	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	Q	17	ARG
14	Q	18	ILE
14	Q	28	VAL
14	Q	32	LEU
14	Q	57	LYS
14	Q	59	LYS
14	Q	65	VAL
14	Q	71	ARG
14	Q	73	LEU
14	Q	83	LYS
14	Q	89	ARG
14	Q	95	HIS
14	Q	101	LEU
14	Q	107	GLU
14	Q	110	LEU
15	R	1	MET
15	R	6	LEU
15	R	8	LYS
15	R	9	LEU
15	R	23	ARG
15	R	27	THR
15	R	30	VAL
15	R	36	GLU
15	R	38	ASN
15	R	41	ARG
15	R	50	ILE
15	R	62	THR
15	R	65	LYS
15	R	74	ARG
15	R	85	LYS
15	R	86	ILE
15	R	88	ILE
15	R	91	ARG
15	R	93	ARG
15	R	99	LEU
15	R	107	ASP
15	R	112	ARG
16	1	8	VAL
16	1	51	LYS
16	1	64	ARG
16	1	74	LEU
16	1	84	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	1	92	ARG
16	1	93	LYS
16	1	95	LEU
16	1	97	ASP
16	1	100	VAL
16	1	101	ARG
16	1	111	GLU
16	1	112	ARG
16	1	114	LYS
17	2	23	GLU
17	2	26	ASP
17	2	28	GLU
17	2	40	LEU
17	2	46	VAL
17	2	49	THR
17	2	52	VAL
17	2	57	VAL
17	2	61	VAL
17	2	68	LYS
17	2	73	SER
17	2	79	VAL
17	2	81	TYR
17	2	83	ARG
17	2	84	LYS
17	2	85	LYS
17	2	89	GLN
17	2	91	TYR
17	2	95	LEU
17	2	100	ARG
18	S	11	ARG
18	S	15	ARG
18	S	20	VAL
18	S	40	ASN
18	S	51	LEU
18	S	52	GLU
18	S	59	VAL
18	S	60	ASN
18	S	65	LEU
18	S	70	TYR
18	S	76	VAL
18	S	94	ASP
18	S	98	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	S	106	ILE
18	S	107	LEU
18	S	111	HIS
18	S	113	LYS
19	T	30	VAL
19	T	45	THR
19	T	63	LYS
19	T	66	LEU
19	T	69	TYR
19	T	75	ASP
19	T	80	ILE
19	T	81	VAL
20	U	2	ARG
20	U	6	HIS
20	U	8	LYS
20	U	13	VAL
20	U	19	LYS
20	U	27	VAL
20	U	29	GLU
20	U	37	VAL
20	U	38	ILE
20	U	39	VAL
20	U	46	LYS
20	U	51	VAL
20	U	54	LYS
20	U	57	GLN
20	U	60	PHE
20	U	61	ILE
20	U	62	GLU
20	U	63	LYS
20	U	75	ILE
20	U	76	CYS
20	U	81	LYS
20	U	84	ARG
20	U	88	LYS
20	U	96	ILE
20	U	97	ARG
20	U	98	VAL
21	V	32	HIS
21	V	42	VAL
21	V	53	ILE
21	V	66	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	V	70	LEU
21	V	71	VAL
21	V	73	GLN
21	V	74	VAL
21	V	85	HIS
21	V	87	ASP
21	V	89	PHE
21	V	107	THR
21	V	117	LEU
21	V	120	ILE
21	V	128	VAL
21	V	144	LEU
21	V	146	ILE
21	V	150	LEU
21	V	154	ASP
21	V	156	LYS
21	V	170	THR
21	V	179	ASP
22	3	12	ASN
22	3	25	ARG
22	3	36	ILE
22	3	50	ASN
23	Z	41	ARG
23	Z	81	LYS
23	Z	82	LEU
23	Z	83	GLU
23	Z	85	LEU
23	Z	90	ILE
24	W	24	LEU
24	W	53	LEU
24	W	65	ASN
25	X	5	LYS
25	X	8	LEU
25	X	9	VAL
25	X	18	ASP
25	X	24	LYS
25	X	36	VAL
25	X	38	GLU
25	X	40	THR
26	4	1	MET
26	4	2	LYS
26	4	9	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	4	14	ILE
26	4	15	ILE
26	4	16	CYS
26	4	18	CYS
26	4	22	ILE
26	4	23	GLU
26	4	24	THR
26	4	27	THR
26	4	32	TYR
26	4	34	GLU
26	4	37	SER
26	4	38	LYS
26	4	39	CYS
26	4	42	PHE
26	4	50	VAL
26	4	51	ASP
26	4	53	GLU
26	4	62	ARG
27	5	15	ARG
27	5	23	HIS
27	5	29	THR
27	5	33	CYS
27	5	35	GLU
27	5	48	GLU
27	5	51	TYR
27	5	56	LYS
28	6	12	GLU
28	6	14	THR
28	6	15	GLU
28	6	17	LYS
28	6	23	THR
28	6	24	GLU
28	6	30	THR
28	6	32	ASN
28	6	37	ARG
28	6	39	TYR
28	6	46	HIS
28	6	50	ARG
28	6	52	VAL
29	7	1	MET
29	7	4	THR
29	7	15	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
29	7	24	THR
29	7	39	ARG
29	7	43	THR
29	7	46	VAL
29	7	47	ARG
29	7	49	ARG
30	8	22	VAL
30	8	23	VAL
30	8	30	ARG
30	8	32	LEU
30	8	40	GLU
30	8	48	PHE
30	8	49	VAL
30	8	52	LYS
30	8	58	ILE
30	8	61	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
3	D	143	HIS
4	E	35	GLN
4	E	55	ASN
4	E	60	ASN
5	F	67	GLN
6	G	41	GLN
10	N	3	GLN
11	O	68	GLN
12	P	45	GLN
16	1	49	HIS
16	1	72	HIS
16	1	81	HIS
17	2	89	GLN
18	S	40	ASN
22	3	35	ASN
25	X	19	GLN
25	X	52	HIS
28	6	46	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2904/2912 (99%)	645 (22%)	39 (1%)
2	B	121/122 (99%)	32 (26%)	0
All	All	3025/3034 (99%)	677 (22%)	39 (1%)

All (677) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	G
1	A	14	A
1	A	15	G
1	A	34	C
1	A	36	G
1	A	46	C
1	A	49	A
1	A	50	U
1	A	51	G
1	A	58	G
1	A	60	G
1	A	71	A
1	A	72	U
1	A	74	A
1	A	75	G
1	A	90	U
1	A	91	A
1	A	93	C
1	A	95	G
1	A	102	G
1	A	118	A
1	A	120	U
1	A	129	C
1	A	140	A
1	A	149	A
1	A	153	C
1	A	154	G
1	A	174	C
1	A	175	G
1	A	181	A
1	A	182	A
1	A	196	A
1	A	199	A
1	A	205	G
1	A	206	U
1	A	214	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	215	G
1	A	216	A
1	A	221	A
1	A	222	A
1	A	225	A
1	A	229	A
1	A	233	A
1	A	241	A
1	A	248	G
1	A	250	G
1	A	252	G
1	A	270(G)	C
1	A	270(K)	C
1	A	270(L)	U
1	A	270(M)	U
1	A	270(O)	U
1	A	270(Q)	C
1	A	271(C)	U
1	A	271	G
1	A	273(D)	C
1	A	274	G
1	A	275	G
1	A	276	A
1	A	279	C
1	A	289	A
1	A	311	A
1	A	324	A
1	A	329	G
1	A	330	A
1	A	333	G
1	A	352	G
1	A	353	G
1	A	355	G
1	A	358	U
1	A	362	U
1	A	363	G
1	A	363(B)	G
1	A	363(E)	U
1	A	363(F)	A
1	A	372	G
1	A	385	C
1	A	386	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	396	G
1	A	405	U
1	A	406	G
1	A	407	G
1	A	411	G
1	A	428	A
1	A	443	A
1	A	444	C
1	A	448	U
1	A	455	C
1	A	457	A
1	A	464	U
1	A	470	A
1	A	480	A
1	A	481	G
1	A	489	G
1	A	504	U
1	A	505	A
1	A	508	G
1	A	509	C
1	A	512	G
1	A	527	C
1	A	529	A
1	A	530	G
1	A	531	C
1	A	532	A
1	A	533	G
1	A	537	C
1	A	547	A
1	A	549	G
1	A	556	G
1	A	563	G
1	A	569	U
1	A	573	G
1	A	575	A
1	A	586	A
1	A	603	A
1	A	607	U
1	A	613	U
1	A	614	U
1	A	615	G
1	A	617	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	621	A
1	A	622	G
1	A	627	A
1	A	634	C
1	A	637	A
1	A	645	C
1	A	646	A
1	A	651	G
1	A	654	A
1	A	654(A)	A
1	A	654(G)	C
1	A	654(H)	G
1	A	654(I)	C
1	A	654(K)	C
1	A	654(L)	G
1	A	654(N)	G
1	A	654(Q)	C
1	A	654(R)	C
1	A	654(T)	A
1	A	669	G
1	A	670	A
1	A	686	G
1	A	708	C
1	A	717	G
1	A	726	G
1	A	730	C
1	A	739	G
1	A	748	G
1	A	753	C
1	A	758	C
1	A	776	G
1	A	779	U
1	A	782	A
1	A	783	A
1	A	784	A
1	A	785	G
1	A	790	C
1	A	792	G
1	A	793	A
1	A	800	A
1	A	805	G
1	A	812	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	819	A
1	A	827	U
1	A	828	U
1	A	832	G
1	A	846	C
1	A	857	C
1	A	859	G
1	A	866	A
1	A	869	G
1	A	878	A
1	A	882	G
1	A	883	G
1	A	885	C
1	A	888	C
1	A	889	C
1	A	890	A
1	A	892	G
1	A	893	C
1	A	894	C
1	A	895	U
1	A	896	A
1	A	897	C
1	A	898	C
1	A	899	A
1	A	901	A
1	A	905	U
1	A	906	G
1	A	907	U
1	A	910	A
1	A	914	C
1	A	915	C
1	A	917	A
1	A	926	A
1	A	932	G
1	A	938	G
1	A	941	A
1	A	945	A
1	A	946	G
1	A	959	A
1	A	961	C
1	A	974	G
1	A	980	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	983	A
1	A	990	A
1	A	996	A
1	A	999	U
1	A	1005	C
1	A	1011	G
1	A	1012	U
1	A	1013	C
1	A	1015	G
1	A	1016	G
1	A	1020	A
1	A	1022	G
1	A	1023	U
1	A	1024	G
1	A	1025	G
1	A	1026	U
1	A	1027	A
1	A	1033	U
1	A	1039	G
1	A	1045	A
1	A	1046	A
1	A	1047	G
1	A	1048	A
1	A	1051	G
1	A	1052	C
1	A	1053	C
1	A	1054	A
1	A	1057	A
1	A	1059	G
1	A	1061	U
1	A	1062	G
1	A	1063	G
1	A	1064	C
1	A	1065	U
1	A	1066	U
1	A	1067	A
1	A	1068	G
1	A	1069	A
1	A	1070	A
1	A	1071	G
1	A	1073	A
1	A	1076	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1079	C
1	A	1082	U
1	A	1083	U
1	A	1086	A
1	A	1087	G
1	A	1088	A
1	A	1089	G
1	A	1091	G
1	A	1092	C
1	A	1094	U
1	A	1095	A
1	A	1096	A
1	A	1098	A
1	A	1099	G
1	A	1105	U
1	A	1112	G
1	A	1122	G
1	A	1126	A
1	A	1129	A
1	A	1130	U
1	A	1135	C
1	A	1136	G
1	A	1142(A)	A
1	A	1143	A
1	A	1149	G
1	A	1155	A
1	A	1160	G
1	A	1170	G
1	A	1173	G
1	A	1174	A
1	A	1175	U
1	A	1176	G
1	A	1177	A
1	A	1178	C
1	A	1180	C
1	A	1204	A
1	A	1205	U
1	A	1220	A
1	A	1236	G
1	A	1247	A
1	A	1253	A
1	A	1255	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1256	G
1	A	1269	A
1	A	1271	G
1	A	1272	A
1	A	1273	U
1	A	1286	A
1	A	1300	U
1	A	1301	A
1	A	1314	C
1	A	1325	G
1	A	1329	U
1	A	1349	A
1	A	1352	U
1	A	1359	A
1	A	1360	A
1	A	1365	A
1	A	1368	G
1	A	1379	A
1	A	1380	G
1	A	1384	A
1	A	1385	G
1	A	1386	C
1	A	1389	G
1	A	1392	A
1	A	1393	A
1	A	1395	A
1	A	1403	C
1	A	1407	C
1	A	1416	G
1	A	1419	A
1	A	1420	U
1	A	1421	G
1	A	1428	C
1	A	1437	C
1	A	1444(A)	A
1	A	1449	A
1	A	1449(A)	G
1	A	1451	C
1	A	1455	G
1	A	1458	C
1	A	1460	A
1	A	1461	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1467	C
1	A	1471	A
1	A	1475	G
1	A	1483	G
1	A	1488	G
1	A	1490	A
1	A	1493	C
1	A	1497	U
1	A	1509	C
1	A	1510	A
1	A	1522	G
1	A	1534	G
1	A	1535	U
1	A	1536	A
1	A	1537	C
1	A	1543	A
1	A	1544	C
1	A	1545	A
1	A	1558	A
1	A	1559	G
1	A	1560	G
1	A	1569	A
1	A	1578	U
1	A	1580	A
1	A	1585	C
1	A	1586	A
1	A	1588	C
1	A	1593	G
1	A	1598	C
1	A	1608	A
1	A	1610	A
1	A	1616	A
1	A	1618	A
1	A	1640	C
1	A	1648	C
1	A	1654	A
1	A	1674	G
1	A	1675	C
1	A	1696	G
1	A	1700	A
1	A	1701	A
1	A	1725	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1728	G
1	A	1729	A
1	A	1730	U
1	A	1731	G
1	A	1742	C
1	A	1743	G
1	A	1756	G
1	A	1758	G
1	A	1762	A
1	A	1763	G
1	A	1764	G
1	A	1773	A
1	A	1780	A
1	A	1782	C
1	A	1791	A
1	A	1800	C
1	A	1801	G
1	A	1802	A
1	A	1816	G
1	A	1820	U
1	A	1829	A
1	A	1834	U
1	A	1835	G
1	A	1839	G
1	A	1847	A
1	A	1848	A
1	A	1858	G
1	A	1869	G
1	A	1871	A
1	A	1878	G
1	A	1888	G
1	A	1889	A
1	A	1900	A
1	A	1906	G
1	A	1912	A
1	A	1913	A
1	A	1914	C
1	A	1917	U
1	A	1929	G
1	A	1930	G
1	A	1931	U
1	A	1936	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1952	A
1	A	1955	U
1	A	1956	U
1	A	1963	U
1	A	1965	C
1	A	1967	C
1	A	1970	A
1	A	1971	A
1	A	1972	A
1	A	1992	G
1	A	1993	U
1	A	1994	C
1	A	2020	A
1	A	2023	G
1	A	2031	A
1	A	2032	G
1	A	2033	A
1	A	2036	C
1	A	2043	C
1	A	2049	G
1	A	2055	C
1	A	2056	G
1	A	2059	A
1	A	2060	A
1	A	2061	G
1	A	2062	A
1	A	2069	G
1	A	2082	A
1	A	2093	G
1	A	2099	U
1	A	2100	G
1	A	2108	C
1	A	2110	G
1	A	2111	C
1	A	2112	G
1	A	2113	U
1	A	2114	A
1	A	2115	G
1	A	2116	G
1	A	2117	A
1	A	2118	U
1	A	2119	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2120	G
1	A	2123	G
1	A	2124	G
1	A	2125	G
1	A	2126	A
1	A	2127	G
1	A	2128	C
1	A	2129	C
1	A	2130	U
1	A	2131	G
1	A	2132	U
1	A	2133	G
1	A	2135	A
1	A	2136	C
1	A	2137	C
1	A	2139	C
1	A	2145	C
1	A	2146	C
1	A	2147	G
1	A	2148	G
1	A	2156	G
1	A	2158	A
1	A	2159	G
1	A	2160	G
1	A	2162	G
1	A	2164	C
1	A	2165	G
1	A	2166	G
1	A	2167	U
1	A	2168	G
1	A	2169	A
1	A	2170	A
1	A	2171	A
1	A	2173	A
1	A	2174	C
1	A	2178	C
1	A	2189	U
1	A	2190	G
1	A	2192	G
1	A	2198	A
1	A	2199	A
1	A	2210	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2211	G
1	A	2212	A
1	A	2213	U
1	A	2215	G
1	A	2225	A
1	A	2226	C
1	A	2238	G
1	A	2239	G
1	A	2245	U
1	A	2275	C
1	A	2280	G
1	A	2283	C
1	A	2287	A
1	A	2288	A
1	A	2297	C
1	A	2305	A
1	A	2307	G
1	A	2308	G
1	A	2309	A
1	A	2321	G
1	A	2325	G
1	A	2334	G
1	A	2335	A
1	A	2336	A
1	A	2342	C
1	A	2345	G
1	A	2346	A
1	A	2347	C
1	A	2350	C
1	A	2354	G
1	A	2383	G
1	A	2385	C
1	A	2392	A
1	A	2394	C
1	A	2401	U
1	A	2402	C
1	A	2403	C
1	A	2406	U
1	A	2410	G
1	A	2411	A
1	A	2420	C
1	A	2424	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2425	A
1	A	2428	G
1	A	2429	G
1	A	2430	A
1	A	2434	A
1	A	2435	A
1	A	2439	A
1	A	2440	C
1	A	2441	C
1	A	2445	G
1	A	2448	A
1	A	2468	G
1	A	2469	A
1	A	2475	C
1	A	2476	A
1	A	2477	C
1	A	2482	G
1	A	2483	C
1	A	2484	G
1	A	2502	G
1	A	2505	G
1	A	2506	U
1	A	2518	A
1	A	2529	G
1	A	2543	G
1	A	2554	U
1	A	2566	A
1	A	2567	G
1	A	2569	G
1	A	2572	A
1	A	2582	G
1	A	2584	U
1	A	2585	U
1	A	2586	C
1	A	2602	A
1	A	2603	G
1	A	2609	U
1	A	2610	C
1	A	2611	U
1	A	2612	C
1	A	2615	U
1	A	2629	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2630	G
1	A	2636	U
1	A	2654	A
1	A	2655	G
1	A	2665	A
1	A	2673	G
1	A	2689	U
1	A	2690	C
1	A	2700	C
1	A	2702	U
1	A	2703	C
1	A	2707	G
1	A	2712(A)	A
1	A	2713	A
1	A	2714	G
1	A	2726	U
1	A	2733	A
1	A	2744	G
1	A	2748	A
1	A	2750	A
1	A	2751	G
1	A	2752	C
1	A	2754	U
1	A	2757	A
1	A	2759	G
1	A	2761	G
1	A	2762	G
1	A	2764	A
1	A	2765	A
1	A	2766	G
1	A	2769	C
1	A	2777	G
1	A	2778	A
1	A	2779	U
1	A	2786	U
1	A	2789	C
1	A	2791	C
1	A	2793	G
1	A	2797	U
1	A	2798	C
1	A	2799	A
1	A	2801	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2802	G
1	A	2805	G
1	A	2809	A
1	A	2810	A
1	A	2812	G
1	A	2818	G
1	A	2820	A
1	A	2821	A
1	A	2833	G
1	A	2834	G
1	A	2835	A
1	A	2860	A
1	A	2872	G
1	A	2879	C
1	A	2880	C
1	A	2892	A
1	A	2893	G
1	A	2894	G
1	A	2896	C
1	A	2897	U
1	A	2902	C
2	B	0	A
2	B	3	C
2	B	4	C
2	B	7	G
2	B	13	A
2	B	15	A
2	B	16	G
2	B	22	U
2	B	24	G
2	B	25	A
2	B	27	C
2	B	30	C
2	B	40	U
2	B	41	U
2	B	42	C
2	B	44	G
2	B	45	A
2	B	53	A
2	B	57	A
2	B	67	G
2	B	73	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	75	G
2	B	76	G
2	B	81	G
2	B	88	C
2	B	89	G
2	B	89(A)	A
2	B	90	C
2	B	101	A
2	B	105	G
2	B	109	G
2	B	115	G

All (39) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	49	A
1	A	128	C
1	A	205	G
1	A	249	C
1	A	278	A
1	A	654(S)	G
1	A	669	G
1	A	752	A
1	A	856	C
1	A	877	U
1	A	888	C
1	A	1022	G
1	A	1066	U
1	A	1085	A
1	A	1088	A
1	A	1171	G
1	A	1300	U
1	A	1427	A
1	A	1460	A
1	A	1558	A
1	A	1653	G
1	A	1819	A
1	A	1912	A
1	A	1913	A
1	A	1955	U
1	A	1992	G
1	A	2191	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2211	G
1	A	2406	U
1	A	2439	A
1	A	2447	G
1	A	2542	A
1	A	2602	A
1	A	2610	C
1	A	2689	U
1	A	2747	G
1	A	2776	A
1	A	2859	G
1	A	2893	G

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	2906/2912 (99%)	-0.34	63 (2%) 59 11	60, 90, 232, 251	0
2	B	122/122 (100%)	0.02	8 (6%) 18 3	91, 127, 154, 200	0
3	D	272/276 (98%)	0.28	15 (5%) 24 4	58, 81, 99, 122	0
4	E	205/206 (99%)	-0.05	5 (2%) 56 9	60, 97, 142, 165	0
5	F	208/210 (99%)	-0.21	2 (0%) 79 23	66, 102, 156, 182	0
6	G	181/182 (99%)	0.10	14 (7%) 13 2	117, 141, 165, 177	0
7	H	170/180 (94%)	0.55	27 (15%) 3 1	146, 200, 223, 235	0
8	K	146/148 (98%)	0.40	11 (7%) 14 2	88, 132, 151, 159	0
9	M	138/140 (98%)	-0.04	7 (5%) 27 4	80, 107, 137, 157	0
10	N	122/122 (100%)	0.79	15 (12%) 5 1	70, 91, 109, 116	0
11	O	150/150 (100%)	0.58	24 (16%) 3 1	66, 105, 140, 179	0
12	P	141/141 (100%)	0.66	17 (12%) 5 1	80, 106, 130, 152	0
13	0	117/118 (99%)	0.19	6 (5%) 27 4	71, 89, 108, 119	0
14	Q	111/112 (99%)	0.69	19 (17%) 2 0	98, 121, 142, 151	0
15	R	137/146 (93%)	-0.03	2 (1%) 70 16	80, 99, 159, 185	0
16	1	117/118 (99%)	-0.52	0 100 100	72, 101, 136, 155	0
17	2	101/101 (100%)	-0.45	0 100 100	71, 123, 139, 148	0
18	S	113/113 (100%)	-0.03	4 (3%) 42 6	68, 83, 113, 161	0
19	T	92/96 (95%)	-0.03	2 (2%) 59 11	77, 94, 118, 128	0
20	U	102/110 (92%)	0.22	4 (3%) 37 5	93, 118, 160, 182	0
21	V	179/206 (86%)	1.74	69 (38%) 1 0	118, 157, 213, 219	0
22	3	77/85 (90%)	0.07	1 (1%) 74 19	74, 95, 111, 151	0
23	Z	97/98 (98%)	0.58	9 (9%) 9 2	67, 91, 135, 157	0
24	W	69/72 (95%)	-0.11	2 (2%) 49 7	90, 112, 133, 164	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	X	59/60 (98%)	0.17	1 (1%) 67 15	79, 102, 145, 162	0
26	4	63/71 (88%)	1.64	22 (34%) 1 0	154, 187, 197, 205	0
27	5	59/60 (98%)	0.14	3 (5%) 27 4	68, 91, 178, 192	0
28	6	45/54 (83%)	2.43	27 (60%) 0 0	138, 164, 181, 183	0
29	7	49/49 (100%)	2.15	21 (42%) 1 0	63, 70, 107, 130	0
30	8	61/65 (93%)	-0.48	0 100 100	73, 87, 106, 121	0
All	All	6409/6523 (98%)	0.02	400 (6%) 20 3	58, 98, 202, 251	0

All (400) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1535	U	15.7
11	O	149	GLU	11.4
1	A	1052	C	11.0
29	7	47	ARG	9.6
11	O	92	GLU	9.6
29	7	48	LYS	8.6
1	A	1051	G	7.7
1	A	1534	G	7.7
21	V	134	PRO	7.5
21	V	162	GLU	7.2
28	6	13	CYS	7.1
21	V	81	ARG	7.0
21	V	2	GLU	6.9
26	4	63	TYR	6.8
21	V	138	GLU	6.7
13	0	101	ALA	6.6
26	4	11	PRO	6.6
21	V	73	GLN	6.6
21	V	72	ARG	6.5
21	V	80	ARG	6.3
8	K	135	GLU	6.3
7	H	81	GLU	6.3
11	O	94	GLU	6.2
26	4	57	GLU	6.2
21	V	51	ALA	6.1
21	V	3	TYR	6.0
29	7	49	ARG	5.9
21	V	50	GLN	5.9
7	H	13	LYS	5.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
28	6	33	LYS	5.7
7	H	127	GLU	5.6
21	V	49	ARG	5.6
4	E	1	MET	5.6
21	V	164	ALA	5.6
28	6	53	LYS	5.5
7	H	126	PRO	5.5
28	6	9	LEU	5.5
1	A	1536	A	5.5
28	6	34	LEU	5.4
1	A	2902	C	5.4
14	Q	108	GLY	5.4
21	V	74	VAL	5.3
21	V	136	PHE	5.3
11	O	150	ALA	5.3
12	P	19	GLY	5.3
21	V	46	LYS	5.3
21	V	75	ASN	5.2
1	A	887	A	5.2
8	K	109	ILE	5.1
11	O	98	GLU	5.1
6	G	83	ARG	5.1
29	7	46	VAL	5.1
11	O	95	VAL	5.1
11	O	96	THR	5.0
11	O	124	LYS	5.0
26	4	55	ARG	5.0
21	V	71	VAL	5.0
7	H	83	TYR	5.0
28	6	29	ASN	5.0
7	H	171	LEU	5.0
1	A	2901	C	4.9
14	Q	84	GLN	4.9
4	E	205	ALA	4.8
12	P	140	ALA	4.7
28	6	31	PRO	4.7
11	O	148	LEU	4.6
21	V	140	ASP	4.6
7	H	170	ARG	4.6
21	V	135	GLU	4.5
28	6	14	THR	4.5
14	Q	79	ALA	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
6	G	152	LEU	4.5
26	4	58	ARG	4.5
3	D	272	ALA	4.4
21	V	142	SER	4.4
29	7	45	ALA	4.3
8	K	41	GLU	4.3
12	P	18	LYS	4.2
14	Q	75	GLU	4.2
6	G	181	ARG	4.2
21	V	70	LEU	4.1
21	V	155	LEU	4.1
7	H	101	ARG	4.1
26	4	49	PHE	4.1
6	G	136	ARG	4.1
2	B	91	C	4.0
23	Z	6	GLU	4.0
25	X	60	GLU	4.0
1	A	2602	A	4.0
10	N	54	GLU	4.0
28	6	32	ASN	4.0
21	V	55	HIS	4.0
21	V	82	ARG	4.0
26	4	60	GLN	4.0
1	A	125	G	3.9
12	P	16	ARG	3.9
1	A	2573	C	3.9
12	P	112	GLU	3.9
14	Q	78	LEU	3.9
10	N	90	GLN	3.9
7	H	29	PRO	3.8
14	Q	76	LYS	3.8
1	A	1533	C	3.8
10	N	120	GLU	3.8
21	V	52	SER	3.7
21	V	99	TYR	3.7
7	H	14	GLY	3.7
26	4	62	ARG	3.7
9	M	87	LEU	3.7
21	V	78	LYS	3.6
21	V	156	LYS	3.6
21	V	141	VAL	3.6
6	G	137	GLU	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
13	0	103	ARG	3.6
26	4	30	GLU	3.6
13	0	100	LEU	3.6
9	M	89	LYS	3.6
12	P	17	LEU	3.6
1	A	2455	G	3.6
26	4	13	ARG	3.6
1	A	961	C	3.6
1	A	4	C	3.6
1	A	46	C	3.5
1	A	774	A	3.5
3	D	68	LYS	3.5
12	P	25	ASP	3.5
28	6	16	CYS	3.5
21	V	79	ARG	3.5
7	H	97	ARG	3.5
1	A	1116	C	3.5
29	7	41	ARG	3.5
21	V	163	LEU	3.5
11	O	123	LEU	3.4
11	O	118	GLY	3.4
21	V	37	VAL	3.4
6	G	118	ARG	3.4
1	A	1026	U	3.4
14	Q	71	ARG	3.4
28	6	12	GLU	3.4
1	A	2368	C	3.4
26	4	59	PHE	3.4
1	A	2126	A	3.4
1	A	2031	A	3.4
26	4	48	ARG	3.4
19	T	33	LYS	3.4
7	H	169	VAL	3.3
20	U	55	TYR	3.3
28	6	52	VAL	3.3
21	V	125	LEU	3.3
5	F	188	ARG	3.3
1	A	1730	U	3.3
12	P	132	VAL	3.3
21	V	96	VAL	3.3
10	N	89	ASN	3.3
21	V	97	GLU	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
26	4	42	PHE	3.3
10	N	101	PRO	3.3
21	V	1	MET	3.3
28	6	50	ARG	3.3
11	O	102	ARG	3.2
26	4	31	ILE	3.2
1	A	1041	C	3.2
1	A	1102	C	3.2
28	6	21	TYR	3.2
14	Q	80	LEU	3.2
26	4	40	HIS	3.2
29	7	44	PRO	3.2
3	D	147	LEU	3.2
21	V	143	GLY	3.2
29	7	32	LYS	3.2
29	7	11	LYS	3.2
9	M	92	ALA	3.2
21	V	128	VAL	3.2
23	Z	13	ILE	3.2
1	A	5	A	3.1
7	H	125	VAL	3.1
29	7	10	ARG	3.1
26	4	29	PRO	3.1
10	N	100	GLY	3.1
18	S	113	LYS	3.1
28	6	51	GLU	3.1
11	O	91	PHE	3.1
2	B	88	C	3.1
10	N	114	ILE	3.1
21	V	54	HIS	3.1
21	V	133	ILE	3.1
1	A	436	C	3.0
7	H	80	SER	3.0
21	V	76	LEU	3.0
26	4	22	ILE	3.0
28	6	20	ASN	3.0
4	E	204	ALA	3.0
20	U	79	CYS	3.0
1	A	1729	A	3.0
14	Q	68	GLN	3.0
14	Q	109	GLY	3.0
13	0	102	GLU	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
11	O	126	VAL	3.0
26	4	61	ARG	3.0
1	A	2028	U	3.0
2	B	90	C	3.0
12	P	136	ALA	3.0
12	P	137	TYR	3.0
21	V	77	ASP	2.9
1	A	47	C	2.9
27	5	56	LYS	2.9
21	V	45	ASP	2.9
7	H	40	GLU	2.9
11	O	147	LEU	2.9
12	P	22	LYS	2.9
21	V	103	ARG	2.9
1	A	856	C	2.9
3	D	182	LEU	2.9
21	V	28	MET	2.9
1	A	2571	C	2.9
1	A	1420	U	2.9
21	V	56	VAL	2.9
1	A	888	C	2.9
2	B	89	G	2.9
21	V	48	PHE	2.9
9	M	10	GLU	2.9
29	7	23	ARG	2.8
12	P	26	TYR	2.8
3	D	271	ILE	2.8
6	G	146	TYR	2.8
3	D	273	ARG	2.8
1	A	685	A	2.8
7	H	124	GLU	2.8
21	V	4	ARG	2.8
4	E	83	ASP	2.8
23	Z	3	LYS	2.8
1	A	1544	C	2.8
1	A	684	G	2.8
29	7	18	PHE	2.8
21	V	98	MET	2.8
21	V	153	SER	2.8
7	H	28	GLY	2.8
7	H	27	LYS	2.8
29	7	14	LYS	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	D	183	ARG	2.8
21	V	152	ALA	2.8
1	A	2900	A	2.7
7	H	99	VAL	2.7
7	H	96	ALA	2.7
10	N	57	VAL	2.7
7	H	98	LEU	2.7
12	P	131	ILE	2.7
9	M	88	GLU	2.7
28	6	43	CYS	2.7
28	6	48	VAL	2.7
21	V	25	PRO	2.7
21	V	53	ILE	2.7
2	B	92	G	2.7
23	Z	60	PHE	2.7
3	D	186	HIS	2.7
21	V	139	VAL	2.7
14	Q	83	LYS	2.7
7	H	102	ALA	2.7
1	A	570	G	2.7
11	O	139	LYS	2.7
8	K	44	LEU	2.7
6	G	138	GLN	2.7
21	V	157	LEU	2.7
13	0	74	LYS	2.7
2	B	78	A	2.6
21	V	5	LEU	2.6
1	A	1053	C	2.6
14	Q	81	GLY	2.6
14	Q	59	LYS	2.6
11	O	88	LEU	2.6
24	W	43	GLN	2.6
29	7	43	THR	2.6
10	N	53	LYS	2.6
18	S	1	MET	2.6
21	V	36	LYS	2.6
19	T	13	LEU	2.6
3	D	67	PHE	2.6
8	K	1	MET	2.6
23	Z	42	GLN	2.6
8	K	138	ILE	2.6
1	A	772	C	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
28	6	18	ARG	2.6
21	V	179	ASP	2.6
1	A	2027	G	2.5
14	Q	20	ARG	2.5
29	7	8	ASN	2.5
14	Q	77	ALA	2.5
9	M	90	MET	2.5
28	6	22	ALA	2.5
23	Z	96	LYS	2.5
12	P	1	MET	2.5
24	W	9	GLN	2.5
28	6	46	HIS	2.4
2	B	103	U	2.4
20	U	58	GLY	2.4
1	A	229	A	2.4
6	G	75	LYS	2.4
28	6	30	THR	2.4
7	H	32	GLU	2.4
1	A	1040	C	2.4
1	A	1055	G	2.4
3	D	250	TRP	2.4
1	A	645	C	2.4
1	A	2367	G	2.4
29	7	1	MET	2.4
1	A	1103	A	2.4
14	Q	58	LEU	2.3
15	R	111	ARG	2.3
6	G	82	LEU	2.3
8	K	43	ASN	2.3
1	A	1117	G	2.3
10	N	36	GLY	2.3
1	A	1128	A	2.3
10	N	98	VAL	2.3
1	A	2506	U	2.3
21	V	126	VAL	2.3
4	E	69	LYS	2.3
3	D	126	GLN	2.3
1	A	2461	C	2.3
12	P	92	GLY	2.3
29	7	20	ALA	2.3
21	V	127	LYS	2.3
8	K	20	ASP	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
28	6	17	LYS	2.3
3	D	148	GLU	2.3
12	P	27	VAL	2.3
6	G	151	ALA	2.3
26	4	43	TYR	2.3
11	O	2	LYS	2.3
28	6	19	ARG	2.3
5	F	69	HIS	2.3
10	N	91	LEU	2.3
21	V	35	ARG	2.2
11	O	119	GLU	2.2
3	D	118	VAL	2.2
21	V	132	ASN	2.2
1	A	1050	A	2.2
6	G	182	LYS	2.2
11	O	103	ALA	2.2
18	S	38	TYR	2.2
18	S	37	ARG	2.2
1	A	2572	A	2.2
13	0	54	LEU	2.2
7	H	77	LYS	2.2
1	A	1100	C	2.2
3	D	175	LEU	2.2
1	A	776	G	2.2
23	Z	72	GLU	2.2
23	Z	95	LEU	2.2
1	A	773	U	2.2
1	A	2489	G	2.2
11	O	145	PRO	2.2
29	7	35	ARG	2.1
11	O	125	VAL	2.1
22	3	85	ALA	2.1
21	V	41	LEU	2.1
26	4	10	VAL	2.1
1	A	1807	G	2.1
1	A	2032	G	2.1
6	G	81	LYS	2.1
10	N	99	PHE	2.1
7	H	30	LYS	2.1
9	M	91	LEU	2.1
28	6	47	THR	2.1
3	D	233	HIS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	686	G	2.1
21	V	24	LEU	2.1
29	7	42	LEU	2.1
7	H	47	GLU	2.1
8	K	2	LYS	2.1
14	Q	74	ALA	2.1
28	6	11	LEU	2.1
10	N	55	GLY	2.1
27	5	55	ARG	2.1
2	B	89(A)	A	2.1
21	V	137	ILE	2.1
29	7	21	ARG	2.1
29	7	24	THR	2.1
6	G	84	LYS	2.1
8	K	108	THR	2.1
1	A	126	A	2.1
10	N	56	ASP	2.1
20	U	51	VAL	2.1
8	K	45	LYS	2.1
11	O	146	VAL	2.1
12	P	133	ARG	2.1
26	4	53	GLU	2.1
14	Q	82	ILE	2.0
21	V	42	VAL	2.0
26	4	12	ALA	2.0
15	R	112	ARG	2.0
21	V	84	GLU	2.0
1	A	775	G	2.0
28	6	36	LEU	2.0
11	O	121	LYS	2.0
27	5	48	GLU	2.0
7	H	95	ARG	2.0
14	Q	111	GLU	2.0
23	Z	15	ALA	2.0
21	V	106	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.